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~~09~~/ 674,350

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NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
NEWS  2            "Ask CAS" for self-help around the clock
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NEWS  5  SEP 01    New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS  6  SEP 27    STANDARDS will no longer be available on STN
NEWS  7  SEP 27    SWETSCAN will no longer be available on STN
NEWS  8  OCT 28    KOREAPAT now available on STN
NEWS  9  NOV 18    Current-awareness alerts, saved answer sets, and current
                   search transcripts to be affected by CERAB, COMPUAB, ELCOM,
                   and SOLIDSTATE reloads

NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS    STN Operating Hours Plus Help Desk Availability
NEWS INTER    General Internet Information
NEWS LOGIN    Welcome Banner and News Items
NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
NEWS WWW      CAS World Wide Web Site (general information)
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 11:11:16 ON 30 NOV 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 11:11:27 ON 30 NOV 2004
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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STRUCTURE FILE UPDATES: 28 NOV 2004 HIGHEST RN 790189-55-8
DICTIONARY FILE UPDATES: 28 NOV 2004 HIGHEST RN 790189-55-8

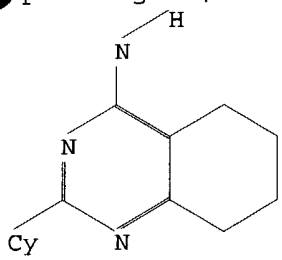
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

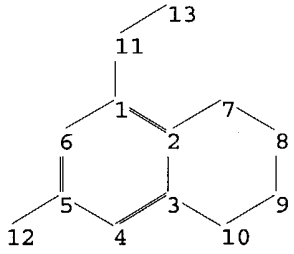
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\10674350.str





chain nodes :
11 12 13
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
1-11 5-12 11-13
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10
exact/norm bonds :
1-11 5-12
exact bonds :
2-7 3-10 7-8 8-9 9-10 11-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
12:Atom 13:CLASS

L1 STRUCTURE UPLOADED

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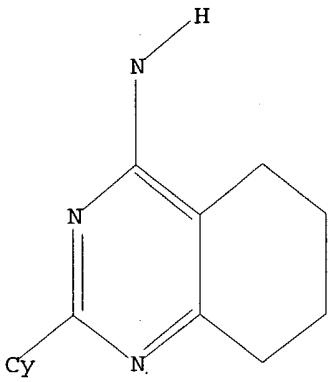
L1 HAS NO ANSWERS
L1 STR

10/ 674,350



Structure attributes must be viewed using STN Express query preparation.

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=> s l1 ful
FULL SEARCH INITIATED 11:11:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   7780 TO ITERATE

100.0% PROCESSED    7780 ITERATIONS                          243 ANSWERS
SEARCH TIME: 00.00.02

L2          243 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   155.42     155.63

FILE 'CAPLUS' ENTERED AT 11:11:53 ON 30 NOV 2004
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FILE COVERS 1907 - 30 Nov 2004  VOL 141 ISS 23
FILE LAST UPDATED: 28 Nov 2004  (20041128/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

=> s l2
L3          48 L2

=> d l3 1- ibib abs hitstr
YOU HAVE REQUESTED DATA FROM 48 ANSWERS - CONTINUE? Y/(N):y
```

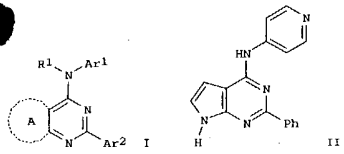
L3 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:857329 CAPLUS
DOCUMENT NUMBER: 141:332209
TITLE: Preparation of bicyclic pyrimidine inhibitors of TGF-β
INVENTOR(S): Dugar, Sundeep; Chakravarty, Sarvajit; Conte, Aurelia; Axon, Jonathan; Mcenroe, Glenn
PATENT ASSIGNEE(S): Scios Inc., USA
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087056	A2	20041014	WO 2004-US9300	20040326

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-458982P P 20030328
GI

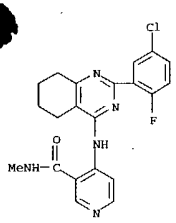


I

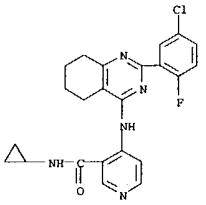
II

AB Title compds. I [R1 = H, (un)substituted-alkyl, -alkenyl, -alkynyl; Ar1 and Ar2 independently = (un)substituted aromatic or heteroarom. moiety; Ring A is (un)substituted, (un)saturated or aromatic and contains 4-7 members, wherein each member independently = C, N, O, or S], as well as their pharmaceutically acceptable salts, are prepared and disclosed as being useful for treating subjects with conditions ameliorated by inhibition of transforming growth factor-β (TGF-β) activity. Thus, e.g., II was prepd by cyclocondensation of benzamidine hydrochloride with Et 2-cyano-4,4-diethoxybutyrate to form 2-phenylpyrrolo[2,3-d]pyrimidone which was chlorinated and substituted with 4-aminopyridine. In TGF-β

RN 773138-92-4 CAPLUS
CN 3-Pyridinecarboxamide, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-methyl- (9CI) (CA INDEX NAME)



RN 773139-03-0 CAPLUS
CN 3-Pyridinecarboxamide, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-cyclopropyl- (9CI) (CA INDEX NAME)



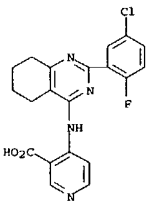
RN 773139-25-6 CAPLUS
CN 3-Pyridinecarboxamide, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-[(2S)-2-hydroxypropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

assays, I were found to possess IC50 values ranging from 0.0145-16.141 μM.

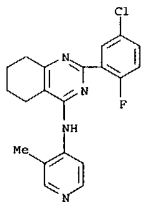
IT **773139-13-2P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of bicyclic pyrimidines as inhibitors of transforming growth factor-β)

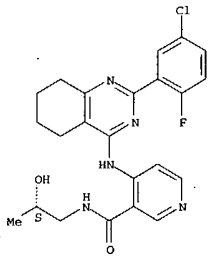
RN 773139-13-2 CAPLUS
CN 3-Pyridinecarboxylic acid, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



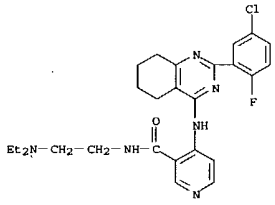
IT **773138-88-8P 773138-92-4P 773139-03-0P 773139-25-6P 773139-29-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of bicyclic pyrimidines as inhibitors of transforming growth factor-β)

RN 773138-88-8 CAPLUS
CN 4-Quinazolinamine, 2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-N-(3-methyl-4-pyridinyl)- (9CI) (CA INDEX NAME)





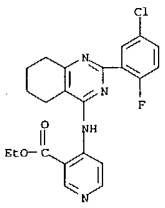
RN 773139-29-0 CAPLUS
CN 3-Pyridinecarboxamide, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-[2-(diethylamino)ethyl]- (9CI) (CA INDEX NAME)



IT **773140-35-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of bicyclic pyrimidines as inhibitors of transforming growth factor-β)

RN 773140-35-5 CAPLUS
CN 3-Pyridinecarboxylic acid, 4-[[2-(5-chloro-2-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L3 ANSWER 2 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:757703 CAPLUS
DOCUMENT NUMBER: 139:255408
TITLE: Azolylaminoazines as inhibitors of protein kinases, and their therapeutic use
INVENTOR(S): Bebbington, David; Binch, Hayley; Charrier, Jean-Damien; Everitt, Simon; Golec, Julian M. C.; Kay, David; Knegtel, Ronald; Miller, Andrew; Pierard, Francoise
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

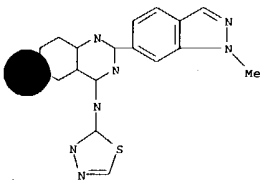
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078427	A1	20030925	WO 2003-US8125	20030314
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004009981	A1	20040115	US 2003-389259	20030314
PRIORITY APPLN. INFO.:			US 2002-364864P P	20020315
OTHER SOURCE(S):	MARPAT 139:255408			

AB The invention discloses azolylaminoazine compds. useful as inhibitors of protein kinases. The invention also discloses pharmaceutically acceptable compns. comprising the compds. and methods of using the compns. in the treatment of various diseases, conditions, or disorders.

IT **603943-83-5**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(azolylaminoazine inhibitors of protein kinases, therapeutic use, and use with other agents)

RN 603943-83-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-methyl-1H-indazol-6-yl)-N-1,3,4-thiadiazol-2-yl- (9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

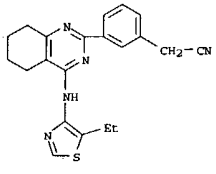
ACCESSION NUMBER: 2003:757702 CAPLUS
DOCUMENT NUMBER: 139:255407
TITLE: Azolylaminoazine compounds as inhibitors of protein kinases, and their therapeutic use
INVENTOR(S): Binch, Hayley; Charrier, Jean-Damien; Everitt, Simon; Golec, Julian M. C.; Kay, David; Knegtel, Ronald; Miller, Andrew; Pierard, Francoise; Bebbington, David
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078426	A1	20030925	WO 2003-US7904	20030314
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004002496	A1	20040101	US 2003-389709	20030314
PRIORITY APPLN. INFO.:			US 2002-364840P P	20020315
			WO 2003-US7904 A	20030314
OTHER SOURCE(S):	MARPAT 139:255407			

AB The invention provides azolylaminoazine compds. useful as inhibitors of protein kinases. The invention also provides pharmaceutically acceptable compns. comprising the compds. and methods of using the compns. in the treatment of various diseases, conditions, and disorders.

IT **603932-46-3**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(azolylaminoazine compds. as inhibitors of protein kinases, therapeutic use, and use with other agents)

RN 603932-46-3 CAPLUS
CN Benzeneacetonitrile, 3-[4-[(5-ethyl-4-thiazolyl)amino]-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)



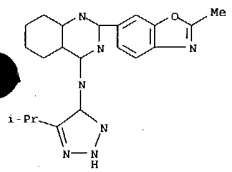
L3 ANSWER 3 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:757527 CAPLUS
DOCUMENT NUMBER: 139:255405
TITLE: Azinylaminoazoles as inhibitors of protein kinases, and their therapeutic use
INVENTOR(S): Bebbington, David; Binch, Hayley; Charrier, Jean-Damien; Everitt, Simon; Golec, Julian M. C.; Kay, David; Knegtel, Ronald; Miller, Andrew; Pierard, Francoise
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003077921	A1	20030925	WO 2003-US7957	20030314
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004009974	A1	20040115	US 2003-389296	20030314
PRIORITY APPLN. INFO.:			US 2002-365003P	P 20020315
OTHER SOURCE(S):	MARPAT 139:255405			

AB The invention provides azinylaminoazole compds. useful as inhibitors of protein kinases. The invention also provides pharmaceutically acceptable compns. comprising the compds. and methods of using the compns. in the treatment of various diseases, conditions, or disorders.
IT **603932-84-9**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(azinylaminoazoles as inhibitors of protein kinases, therapeutic use, and use with other agents)
RN 603932-84-9 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(2-methyl-6-benzoxazolyl)-N-[5-(1-methylethyl)-2H-1,2,3-triazol-4-yl]- (9CI) (CA INDEX NAME)

L3 ANSWER 4 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:472388 CAPLUS
DOCUMENT NUMBER: 139:53030
TITLE: Pyrimidine-based and quinazoline-based compounds useful as GSK-3 inhibitors
INVENTOR(S): Choquette, Deborah; Davies, Robert J.; Wannamaker, Marion W.
PATENT ASSIGNEE(S): Vertex Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003049739	A1	20030619	WO 2002-US39190	20021209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003199526	A1	20031023	US 2002-314905	20021209
EP 1474147	A1	20041110	EP 2002-799913	20021209
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PRIORITY APPLN. INFO.:			US 2001-338857P	P 20011207
			WO 2002-US39190	W 20021209
OTHER SOURCE(S):	MARPAT 139:53030			

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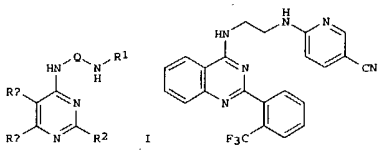
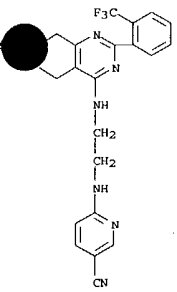


AB The invention provides a compound of formula I or a pharmaceutically acceptable derivative thereof [wherein: R1 = (un)substituted 5- to 6-membered monocyclic or 8- to 10-membered bicyclic (hetero)aryl with 0-4 N/O/S atom(s); Q = (un)substituted C1-4 alkylene chain with 0-2 non-adjacent CH2 optionally replaced by SO2 or CO; R2 = certain (un)substituted Ph, thienyl, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ra, Rb = -T-R3; or RaRb = atoms to complete fused, partially saturated or aromatic, 5- to 8-membered ring with 0-3 N/O/S atom(s) and

L3 ANSWER 5 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
optionally substituted by oxo, -T-R3, etc.; T = bond or C1-4 alkylene chain; R3 = H, halo, OH or derivs., NH2 or derivs., CN, SH or derivs., CHO or derivs., CO2H or derivs., etc.; including pharmaceutically acceptable derivs. and prodrugs]. The compds. are inhibitors of protein kinases, particularly GSK-3 (glycogen synthase kinase 3) mammalian protein kinases. The invention also provides pharmaceutically acceptable compns. comprising the compds. of the invention, and methods of utilizing the compds. and compns. in the treatment of various protein kinase-mediated disorders, such as diabetes, cancer, stroke, and Alzheimer's disease. A table of over 200 compds. I is given in claims. Prepns. of 37 compds. are described in detail. For instance, 4-chloro-2-(2-trifluoromethylphenyl)quinazoline was thermally condensed with 6-(2-aminoethylamino)nicotinonitrile (neat, approx. 140°) to give 49% title compd. II. In a test for inhibition of GSK-3β in vitro, 17 compds. I, including II, had Ki < 0.1 μM, and 16 compds. had Ki of 0.1 to 1.0 μM.

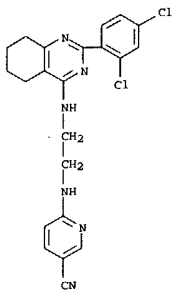
IT **544677-63-6P**, 6-[2-[2-(2-Trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-ylamino]ethylamino]nicotinonitrile **544677-64-7P 544677-65-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidine-based compds. useful as GSK-3 inhibitors)

RN 544677-63-6 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[[2-[[5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]-4-quinazolinyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

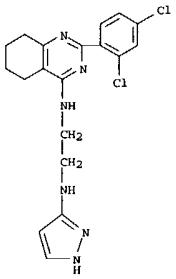


RN 544677-64-7 CAPLUS
CN 3-Pyridinecarbonitrile, 6-[[2-[[2-(2,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 5 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 544677-65-8 CAPLUS
CN 1,2-Ethanediamine, N-[2-(2,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]-N'-1H-pyrazol-3-yl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:220584 CAPLUS
DOCUMENT NUMBER: 136:247584
TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Bebbington, David; Knegtel, Ronald; Golec, Julian M. C.; Li, Pan; Davies, Robert; Charrier, Jean-Damien
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 356 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022608	A1	20020321	WO 2001-US42152	20010914
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2422380	AA	20020321	CA 2001-2422380	20010914
AU 2001096871	A5	20020326	AU 2001-96871	20010914
US 2003055044	A1	20030320	US 2001-953505	20010914
US 6638926	B2	20031028		
US 2003064981	A1	20030403	US 2001-952836	20010914
US 6613776	B2	20030902		
US 2003064982	A1	20030403	US 2001-952875	20010914
US 2003073687	A1	20030417	US 2001-952671	20010914
US 6660731	B2	20031209		
US 2003078166	A1	20030424	US 2001-955601	20010914
US 6696452	B2	20040224		
US 2003083327	A1	20030501	US 2001-952833	20010914
US 6610677	B2	20030826		
EP 1317452	A1	20030611	EP 2001-977779	20010914
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ZA 2003001701	A	20040301	ZA 2003-1701	20010914
ZA 2003001703	A	20040302	ZA 2003-1703	20010914
JP 2004509118	T2	20040325	JP 2002-526861	20010914
US 2004097501	A1	20040520	US 2001-953471	20010914
CA 2432303	AA	20020829	CA 2001-2432303	20011219
CA 2432223	AA	20020906	CA 2001-2432223	20011219
EP 1345922	A1	20030924	EP 2001-271061	20011219
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EP 1355905	A1	20031029	EP 2001-273861	20011219
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NZ 526472	A	20040430	NZ 2001-526472	20011219
JP 2004518743	T2	20040624	JP 2002-565976	20011219
JP 2004519479	T2	20040702	JP 2002-567928	20011219
ZA 2003001697	A	20040301	ZA 2003-1697	20030228
ZA 2003001699	A	20040301	ZA 2003-1699	20030228

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

ZA 2003001702	A	20040301	ZA 2003-1702	20030228
ZA 2003001704	A	20040301	ZA 2003-1704	20030228
ZA 2003001698	A	20040302	ZA 2003-1698	20030228
NO 2003001188	A	20030513	NO 2003-1188	20030314
NO 2003002704	A	20030821	NO 2003-2704	20030613
US 2004224944	A1	20041111	US 2003-624800	20030722
US 2004116454	A1	20040617	US 2003-692355	20031023
US 2004157893	A1	20040812	US 2003-722374	20031125
US 2004132781	A1	20040708	US 2003-736426	20031215
US 2004167141	A1	20040826	US 2004-775699	20040210

PRIORITY APPLN. INFO.:

US 2000-232795P	P	20000915
US 2000-257887P	P	20001221
US 2001-286949P	P	20010427
US 2001-952671	A3	20010914
US 2001-955601	A3	20010914
WO 2001-US42152	W	20010914
US 2001-26966	A1	20011219
WO 2001-US49139	W	20011219
WO 2001-US50312	W	20011219
US 2001-34019	A3	20011220
US 2001-34683	A1	20011220

OTHER SOURCE(S): MARPAT 136:247584
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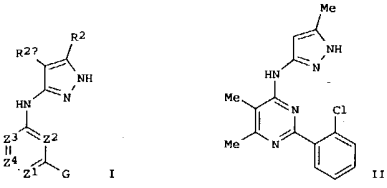
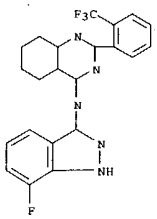


AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliphatic), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliphatic group; or N(R6)2 = heterocyclyl

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (pyrimidinyl)pyrazolamines and indazolamines I [wherein Z1 = CR9; Z2 and Z3 = N; Z4 = CRy]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

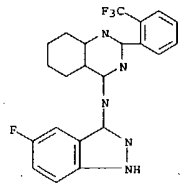
IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine, **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404826-35-3 CAPLUS

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Quinazolinamine, N-(5-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



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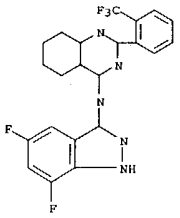

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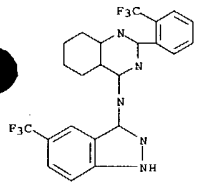
RN 404826-37-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(trifluoromethyl)-1H-indazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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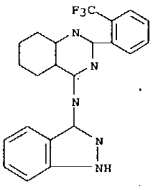

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404828-08-6 CAPLUS
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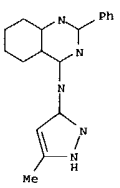
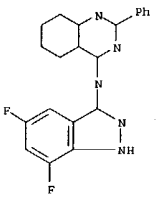


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404829-09-0 CAPLUS

L3 ANSWER 6 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404829-10-3 CAPLUS
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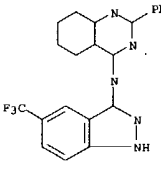

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220583 CAPLUS
DOCUMENT NUMBER: 136:247583
TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Davies, Robert; Bebbington, David; Knegtel, Ronald; Wannamaker, Marion; Li, Pan; Forester, Cornelia; Pierce, Albert; Kay, David
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 373 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022607	A1	20020321	WO 2001-US28940	20010914
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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US 6638926	B2	20031028		
US 2003064981	A1	20030403	US 2001-952836	20010914
US 6613776	B2	20030902		
US 2003064982	A1	20030403	US 2001-952875	20010914
US 2003073687	A1	20030417	US 2001-952671	20010914
US 6660731	B2	20031209		
US 2003078166	A1	20030424	US 2001-955601	20010914
US 6696452	B2	20040224		
US 2003083327	A1	20030501	US 2001-952833	20010914
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EP 1318997	A1	20030618	EP 2001-971082	20010914
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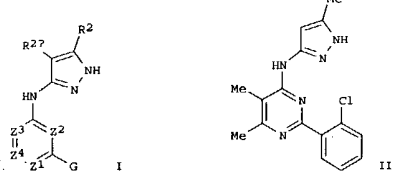


I II

AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO,

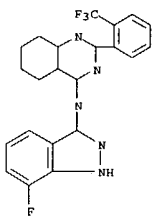
L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliph., (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliph.), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliph.), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliph. group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (pyrimidinyl)pyrazolamines and indazolamines I [wherein Z1 and Z2 = N; Z3 = CRx; Z4 = CRy; G = Ring C]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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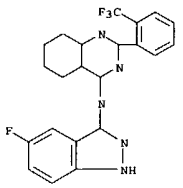

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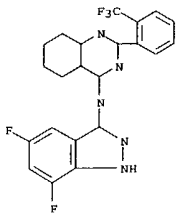
L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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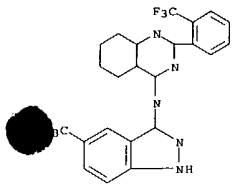

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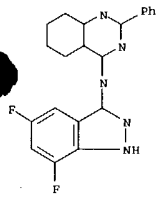
L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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RN 404829-10-3 CAPLUS
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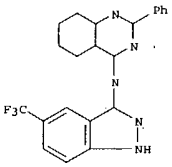

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
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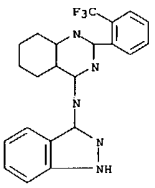
L3 ANSWER 7 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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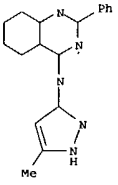

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L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220582 CAPLUS
DOCUMENT NUMBER: 136:247582
TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Bebbington, David; Binch, Hayley; Knegtel, Ronald; Golec, Julian M. C.; Patel, Sanjay; Charrier, Jean-Damien; Kay, David; Davies, Robert; Li, Pan; Wannamaker, Marion; Forster, Cornelia; Pierce, Albert
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 355 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

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L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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US 2004157893	A1	20040812	US 2003-722374		20031125
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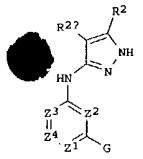
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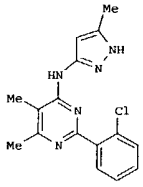
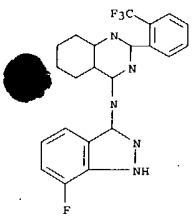

II

AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliph.), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliph.), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliph. group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (pyrimidinyl)pyrazolamines and indazolamines I [wherein Z1 and Z2 = N; Z3 = CRx; Z4 = CRy; G = Ring D]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)(2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)(2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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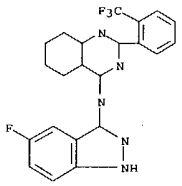
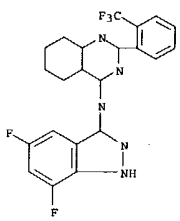


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-36-4 CAPLUS
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

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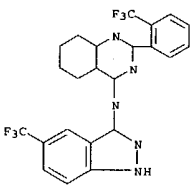

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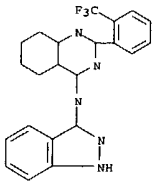

L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404828-08-6 CAPLUS
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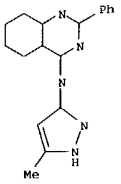

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RN 404829-09-0 CAPLUS
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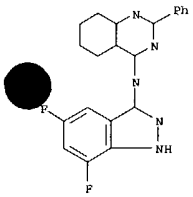

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RN 404829-10-3 CAPLUS
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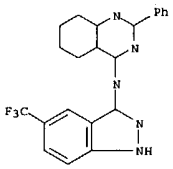
L3 ANSWER 8 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:220581 CAPLUS
DOCUMENT NUMBER: 136:247581
TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Golec, Julian M. C.; Charrier, Jean-Damien; Knegtel, Ronald; Bebbington, David; Davies, Robert; Li, Pan
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 357 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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US 6660731	B2	20031209		
US 2003078166	A1	20030424	US 2001-955601	20010914
US 6696452	B2	20040224		
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EP 1317449	A1	20030611	EP 2001-973050	20010914
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L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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PRIORITY APPLN. INFO.:

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US 2001-286949P	P	20010427
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WO 2001-US28793	W	20010914
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WO 2001-US49139	W	20011219
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US 2001-34019	A3	20011220
US 2001-34683	A1	20011220

OTHER SOURCE(S): MARPAT 136:247581
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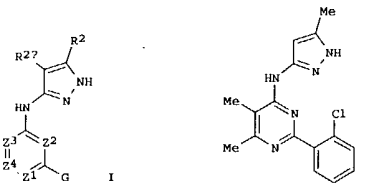


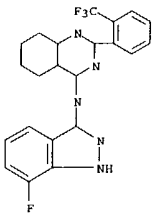
AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliphatic), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliphatic group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepared as protein kinase inhibitors, especially as

L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover pyrazolamines and indazolamines I [wherein Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N; at least one of Z1 or Z3 = N]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-35-3 CAPLUS
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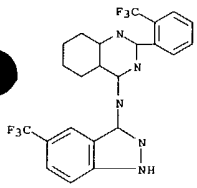
L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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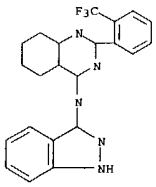

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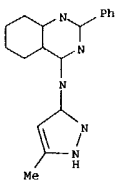

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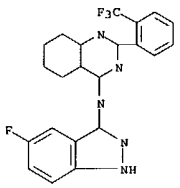
RN 404829-09-0 CAPLUS

L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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RN 404826-36-4 CAPLUS
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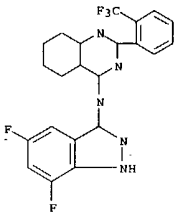
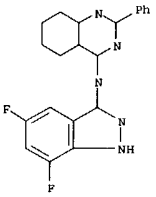


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-37-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(trifluoromethyl)-1H-indazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404829-10-3 CAPLUS
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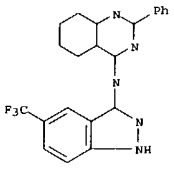

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220580 CAPLUS
DOCUMENT NUMBER: 136:247606
TITLE: Preparation of 3-(4-pyrimidinylamino)pyrazole derivatives as protein kinase inhibitors, especially of Aurora-2 and GSK-3, for treating cancer, diabetes and Alzheimer's disease.
INVENTOR(S): Davies, Robert; Bebbington, David; Binch, Haley; Knegtel, Ronald; Golec, Julian M. C.; Patel, Sanjay; Charrier, Jean-Damien; Kay, David; Davies, Robert
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 357 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

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EP 1345922	A1	20030924	EP 2001-271061	20011219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
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L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

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PRIORITY APPLN. INFO.:

US 2000-232795P	P	20000915
US 2000-257887P	P	20001221
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US 2001-26966	A1	20011219
WO 2001-US49139	W	20011219
WO 2001-US50312	W	20011219
US 2001-34019	A3	20011220
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OTHER SOURCE(S): MARPAT 136:247606
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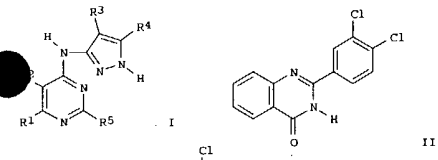
L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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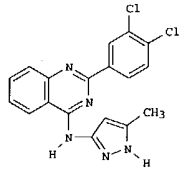
II



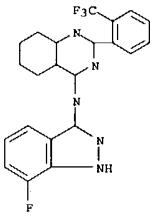
III

AB The preparation of title compds. I and their pharmaceutically acceptable salts or prodrugs is described [wherein: R1, R2 = dependently form (un)substituted fused, unsatd. or partially unsatd., 5-8 membered carbocyclo ring; R3, R4 = independently H, aliphatic, aryl, heteroaryl, heterocyclyl, or wide variety of functionalized sidechains; or dependently form a fused, 5-8 membered, unsatd. or partially unsatd. ring having 0-3 ring heteroatoms (N, S, O); R5 = fused, (un)substituted 5-7 membered monocyclic ring or 8-10 membered bicyclic ring (aryl, heteroaryl, heterocyclyl or carbocyclyl, said heteroaryl or heterocyclyl ring having 1-4 ring heteroatoms (N, S, O))]. For example, chlorination of quinazolone II with phosphorus oxychloride, followed by condensation with 3-amino-5-methylpyrazole afforded claimed compound III. Compds. I are inhibitors of GSK-3 and Aurora-2 protein kinases. The invention also relates to methods of treating diseases associated with these protein kinases, such as diabetes, cancer and Alzheimer's disease. In bioassays, compds. I inhibited the following kinases with Kis reported < 100 nM: GSK-3β (163 compds.), AURORA-2 (65 compds.), CDK-2 (no data), ERK2 (8 compds.), AKT (no data), and Human Src kinase (21 compds.). Claims included 146 specific compds., and 188 examples were given. The syntheses of 6 compds. and 46 intermediates are described.

IT **404826-34-2P 404826-35-3P 404826-36-4P**
404826-37-5P 404826-44-4P 404828-08-6P
404844-78-6P 404844-81-1P 404844-87-7P
404845-05-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(4-pyrimidinylamino)pyrazole compds. as protein kinase inhibitors)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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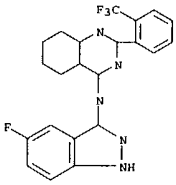

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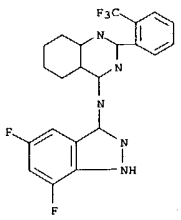
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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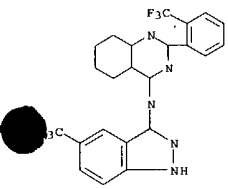

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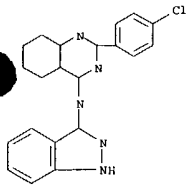
RN 404826-44-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-1H-indazol-3-yl-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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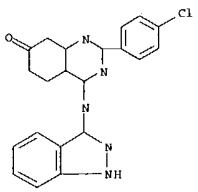

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RN 404844-87-7 CAPLUS
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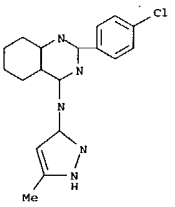

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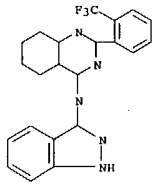
L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
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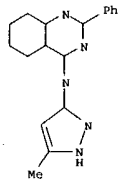

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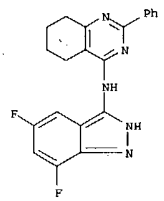
RN 404844-78-6 CAPLUS
CN 4-Quinazolinamine, 2-(4-chlorophenyl)-5,6,7,8-tetrahydro-N-1H-indazol-3-yl- (9CI) (CA INDEX NAME)

L3 ANSWER 10 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 404845-05-2 CAPLUS
CN 4-Quinazolinamine, N-(5,7-difluoro-2H-indazol-3-yl)-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220579 CAPLUS
DOCUMENT NUMBER: 136:247580
TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Davies, Robert; Li, Pan; Golec, Julian; Bebbington, David
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 406 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022603	A1	20020321	WO 2001-US28738	20010914
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US 2003064981	A1	20030403	US 2001-952836	20010914
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US 2003078166	A1	20030424	US 2001-955601	20010914
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CA 2432303	AA	20020829	CA 2001-2432303	20011219
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L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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US 2004167141	A1	20040826	US 2004-775699	20040210
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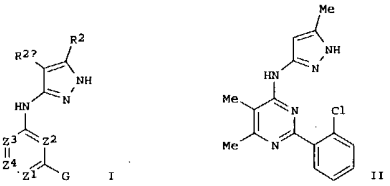
			US 2001-34683	A1 20011220

OTHER SOURCE(S): MARPAT 136:247580
GI



I II

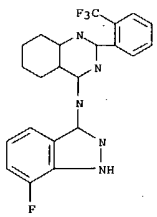
AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR,

L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliph.), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliph.), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliph. group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (triazinyl)pyrazolamines and indazolamines I [wherein Z1, Z2, and Z3 = N; Z4 = CRy]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 404826-35-3 CAPLUS
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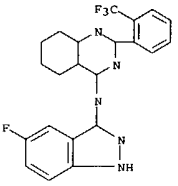

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-36-4 CAPLUS
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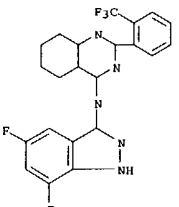

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RN 404826-37-5 CAPLUS
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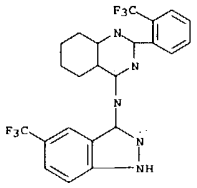
L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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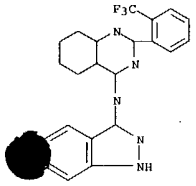
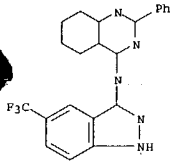


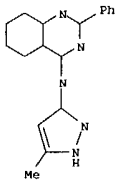
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404828-08-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(5-methyl-1H-pyrazol-3-yl)-2-phenyl- (9CI) (CA INDEX NAME)

L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 11 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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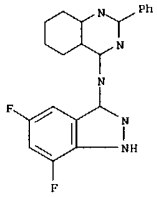
RN 404829-09-0 CAPLUS
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



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RN 404829-10-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-phenyl-N-[5-(trifluoromethyl)-1H-indazol-3-yl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220578 CAPLUS
DOCUMENT NUMBER: 136:263164
TITLE: Preparation of triazolamines as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease
INVENTOR(S): Bebbington, David; Knegtel, Ronald; Binch, Haley; Golec, Julian M. C.; Li, Pan; Charrier, Jean-Damien
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 377 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 14
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022602	A2	20020321	WO 2001-US42162	20010914
WO 2002022602	A3	20020627		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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US 6638926	B2	20031028		
US 2003064981	A1	20030403	US 2001-952836	20010914
US 6613776	B2	20030902		
US 2003064982	A1	20030403	US 2001-952875	20010914
US 2003073687	A1	20030417	US 2001-952671	20010914
US 6660731	B2	20031209		
US 2003078166	A1	20030424	US 2001-955601	20010914
US 6696452	B2	20040224		
US 2003083327	A1	20030501	US 2001-952833	20010914
US 6610677	B2	20030826		
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US 2004097501	A1	20040520	US 2001-953471	20010914
CA 2432303	AA	20020829	CA 2001-2432303	20011219
CA 2432223	AA	20020906	CA 2001-2432223	20011219
EP 1345922	A1	20030924	EP 2001-271061	20011219
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L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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US 2004116454	A1	20040617	US 2003-692355		20031023
US 2004157893	A1	20040812	US 2003-722374		20031125
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			US 2001-955601	A3	20010914
			WO 2001-US42162	W	20010914
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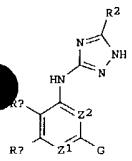
			WO 2001-US50312	W	20011219
			US 2001-34019	A3	20011220
			US 2001-34683	A1	20011220

OTHER SOURCE(S): MARPAT 136:263164
GI



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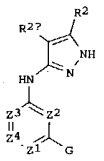

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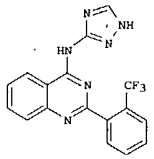


III

AB Triazolamines I and pyrazolamines II [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or

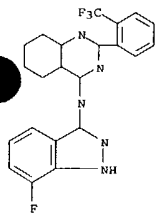
L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)satd. fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring contg. 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliph., (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliph.), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliph.), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliph. group, or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (heterocyclyl)triazolamines I [wherein Z1 = N or CR9; Z2 = N or CH; R9 is defined above]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-quinazolinyl)-1H-1,2,4-triazol-3-amine III was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 1.0-20 μM for Aurora-2.

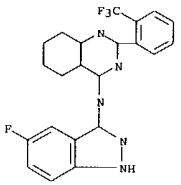
IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine **404889-04-9P 404889-05-0P 404889-06-1P 404889-07-2P 404889-08-3P 404889-14-1P 404891-16-3P 404891-24-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of triazolamines, pyrazolamines, and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 404826-35-3 CAPLUS
CN 4-Quinazolinamine, N-(5-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



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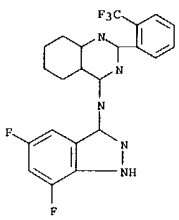
RN 404826-36-4 CAPLUS
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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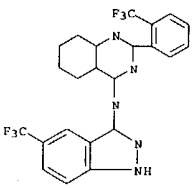
RN 404826-37-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(trifluoromethyl)-1H-indazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



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RN 404826-44-4 CAPLUS
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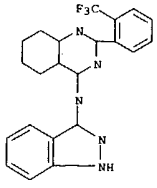

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
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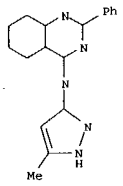
RN 404828-08-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(5-methyl-1H-pyrazol-3-yl)-2-phenyl- (9CI) (CA INDEX NAME)



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RN 404829-09-0 CAPLUS
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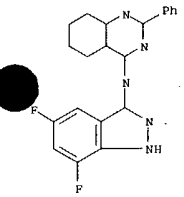

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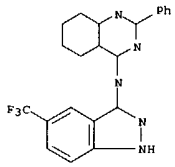
RN 404829-10-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-phenyl-N-[5-(trifluoromethyl)-1H-indazol-3-yl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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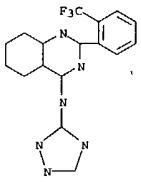

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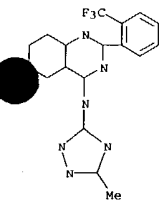
L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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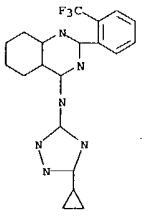
CN 4-Quinazolinamine, N-(5-cyclopropyl-1H-1,2,4-triazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



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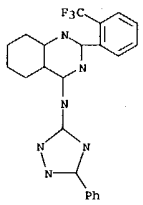
RN 404889-07-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(5-phenyl-1H-1,2,4-triazol-3-yl)-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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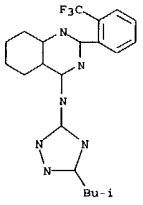
RN 404889-08-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(2-methylpropyl)-1H-1,2,4-triazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



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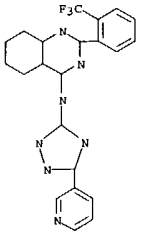
RN 404889-14-1 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(3-pyridinyl)-1H-1,2,4-triazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



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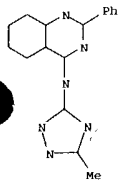
RN 404891-16-3 CAPLUS

CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(5-methyl-1H-1,2,4-triazol-3-yl)-2-phenyl- (9CI) (CA INDEX NAME)

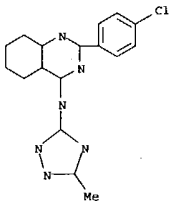


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404891-24-3 CAPLUS

CN 4-Quinazolinamine, 2-(4-chlorophenyl)-5,6,7,8-tetrahydro-N-(5-methyl-1H-1,2,4-triazol-3-yl)- (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:220577 CAPLUS

DOCUMENT NUMBER: 136:247579

TITLE: Preparation of pyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease

INVENTOR(S): Knegtel, Ronald; Bebbington, David; Binch, Hayley; Golec, Julian; Patel, Sanjay; Charrier, Jean-Damien; Kay, David; Davies, Robert; Li, Pan; Wannamaker, Marion; Forster, Cornelia; Pierce, Albert

PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA

SOURCE: PCT Int. Appl., 376 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 14

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022601	A1	20020321	WO 2001-US28740	20010914
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2422354	AA	20020321	CA 2001-2422354	20010914
AU 2001090914	A5	20020326	AU 2001-90914	20010914
US 2003055044	A1	20030320	US 2001-953505	20010914
US 6638926	B2	20031028		
US 2003064981	A1	20030403	US 2001-952836	20010914
US 6613776	B2	20030902		
US 2003064982	A1	20030403	US 2001-952875	20010914
US 2003073687	A1	20030417	US 2001-952671	20010914
US 6660731	B2	20031209		
US 2003078166	A1	20030424	US 2001-955601	20010914
US 6696452	B2	20040224		
US 2003083327	A1	20030501	US 2001-952833	20010914
US 6610677	B2	20030826		
EP 1317444	A1	20030611	EP 2001-970971	20010914
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
ZA 2003001701	A	20040301	ZA 2003-1701	20010914
ZA 2003001703	A	20040302	ZA 2003-1703	20010914
JP 2004509113	T2	20040325	JP 2002-526854	20010914
US 2004097501	A1	20040520	US 2001-953471	20010914
CA 2432303	AA	20020829	CA 2001-2432303	20011219
CA 2432223	AA	20020906	CA 2001-2432223	20011219
EP 1345922	A1	20030924	EP 2001-271061	20011219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
EP 1355905	A1	20031029	EP 2001-273861	20011219
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NZ 526472	A	20040430	NZ 2001-526472	20011219
JP 2004518743	T2	20040624	JP 2002-565976	20011219
JP 2004519479	T2	20040702	JP 2002-567928	20011219

L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

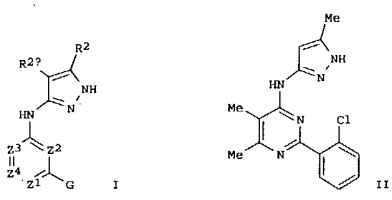
ZA 2003001697	A	20040301	ZA 2003-1697	20030228
ZA 2003001699	A	20040301	ZA 2003-1699	20030228
ZA 2003001702	A	20040301	ZA 2003-1702	20030228
ZA 2003001704	A	20040301	ZA 2003-1704	20030228
ZA 2003001698	A	20040302	ZA 2003-1698	20030228
NO 2003002704	A	20030821	NO 2003-2704	20030613
US 2004224944	A1	20041111	US 2003-624800	20030722
US 2004116454	A1	20040617	US 2003-692355	20031023
US 2004157893	A1	20040812	US 2003-722374	20031125
US 2004132781	A1	20040708	US 2003-736426	20031215
US 2004167141	A1	20040826	US 2004-775699	20040210

PRIORITY APPLN. INFO.:

US 2000-232795P	P	20000915
US 2000-257887P	P	20001221
US 2001-286949P	P	20010427
US 2001-952671	A3	20010914
US 2001-955601	A3	20010914
WO 2001-US28740	W	20010914
US 2001-26966	A1	20011219
WO 2001-US49139	W	20011219
WO 2001-US50312	W	20011219
US 2001-34019	A3	20011220
US 2001-34683	A1	20011220

OTHER SOURCE(S): MARPAT 136:247579

GI

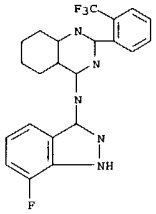


AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un)substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR6OCO, CR6OCONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6)2NR6NR6, C(R6)2NR6SO2NR6, C(R6)2NR6CONR6, or CONR6; R = H or (un)substituted aliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, S00-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliphatic), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un)substituted aliphatic group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR,

L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
COR, CO2R, COCOR, etc.] were prepd. as protein kinase inhibitors, esp. as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover pyrimidinyl- and pyridinyl- pyrazolamines and indazolamines I [wherein Z1 = N, CRa, or CH; Z2 = N or CH; and at least one of Z1 or Z2 = N; Z3 = CRx; Z4 = CRy; Ra = halo, OR, COR, CO2R, COCOR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, etc.; R and R4 are defined above]. Examples include data for approx. 300 invention compds. prepd. by a variety of synthetic methods and bioassay results for the inhibition of GSK-β3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepd. and exhibited Ki values of < 0.1 μM for glycogen synthetase kinase 3β (GSK-3β) and 0.1-1.0 μM for Aurora-2.

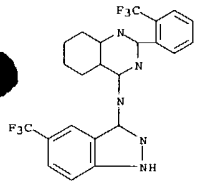
IT **404826-34-2P**, (7-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-35-3P**, (5-Fluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-36-4P**, (5,7-Difluoro-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-37-5P**, (5-Trifluoromethyl-1H-indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404826-44-4P**, (1H-Indazol-3-yl)[2-(2-trifluoromethylphenyl)-5,6,7,8-tetrahydroquinazolin-4-yl]amine **404828-08-6P**, (5-Methyl-2H-pyrazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-09-0P**, (5,7-Difluoro-1H-indazol-3-yl)(2-phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)amine **404829-10-3P**, (2-Phenyl-5,6,7,8-tetrahydroquinazolin-4-yl)(5-trifluoromethyl-1H-indazol-3-yl)amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404826-34-2 CAPLUS
CN 4-Quinazolinamine, N-(7-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



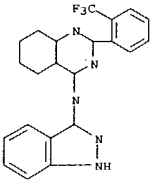
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-44-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-1H-indazol-3-yl-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404828-08-6 CAPLUS
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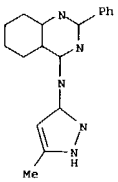
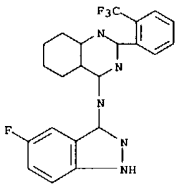


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404829-09-0 CAPLUS

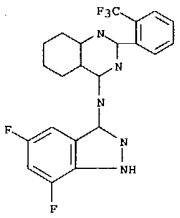
L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 404826-35-3 CAPLUS
CN 4-Quinazolinamine, N-(5-fluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-36-4 CAPLUS
CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

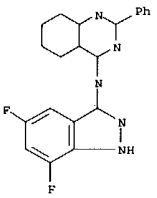


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404826-37-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[5-(trifluoromethyl)-1H-indazol-3-yl]-2-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

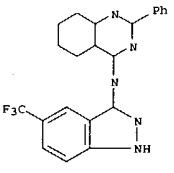
L3 ANSWER 13 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CN 4-Quinazolinamine, N-(5,7-difluoro-1H-indazol-3-yl)-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 404829-10-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-phenyl-N-[5-(trifluoromethyl)-1H-indazol-3-yl]- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 14 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:158388 CAPLUS
DOCUMENT NUMBER: 136:200203
TITLE: Preparation of 4-aminoquinazolines for use in inhibiting neoplastic cells and related conditions
INVENTOR(S): Pamukcu, Rifat; Piazza, Gary
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp., Cont. of U.S. Ser. No. 60,444, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002025968	A1	20020228	US 2001-952769	20010914
			US 1998-60444	B1 19980415

PRIORITY APPLN. INFO.:
OTHER SOURCE(S): MARPAT 136:200203
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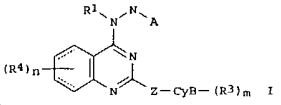

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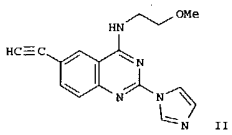


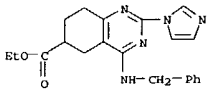
II

AB Title compds. I [wherein R1 = H or alkyl; Y = alkylene; A = ORa or S(O)pRa; Ra = alkylhydroxy; p = 0-2; Z = single bond, methylene, ethylene, vinylene, or ethynylene; CyB = heterocyclic ring; R3 = H, alkyl, alkoxy, halo, or CF3; R4 = H, alkyl, alkoxy, CO2H, carboxy ester, alkanoylamino, alkylsulfonylamino, alkylthio, alkylsulfinyl, alkylsulfonyl, ethynyl, hydroxymethyl, acetyl, or (un)substituted sulfamoyl, carbamoyl, etc.; m and n = independently 1-2; or pharmaceutically acceptable salts or hydrates thereof] were prepared for inhibiting neoplastic cells and related conditions. For example, amination of 2,4-dichloro-6-(2-triethylsilylethynyl)quinazolin-2,4-dione (preparation given) with

2-methoxyethylamine in CHCl3, followed by addn. of imidazole in EtOH and deprotection using NBu4F, afforded II. I are useful in the treatment of precancerous and cancerous lesions, including malignant melanomas, breast cancer, and colon cancer (no data).

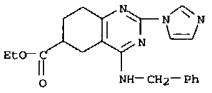
IT **157863-78-0P**, 6-Ethoxycarbonyl-4-Phenylmethylamino-2-(1-Imidazolyl)-5,6,7,8-Tetrahydroquinazoline
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(antineoplastic agent; preparation of aminoquinazolines for use in inhibiting neoplastic cells and related conditions)

RN 157863-78-0 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



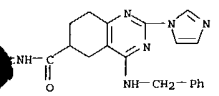
IT **157863-79-1P**, 6-Ethoxycarbonyl-4-Phenylmethylamino-2-(1-Imidazolyl)-5,6,7,8-Tetrahydroquinazoline dihydrochloride
157863-80-4P, 6-Ethylaminocarbonyl-4-Phenylmethylamino-2-(1-Imidazolyl)-5,6,7,8-Tetrahydroquinazoline Dihydrochloride
157863-88-2P, 6-Carboxy-4-Phenylmethylamino-2-(1-Imidazolyl)-5,6,7,8-Tetrahydroquinazoline Sodium Salt **171661-65-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antineoplastic agent; preparation of aminoquinazolines for use in inhibiting neoplastic cells and related conditions)

RN 157863-79-1 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)



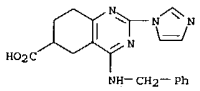
●2 HCl

RN 157863-80-4 CAPLUS
CN 6-Quinazolinecarboxamide, N-ethyl-5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



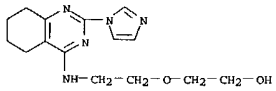
●2 HCl

RN 157863-88-2 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)



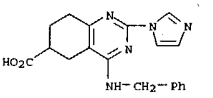
● Na

RN 171661-65-7 CAPLUS
CN Ethanol, 2-[2-[[5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-quinazolinyl]amino]ethoxy]- (9CI) (CA INDEX NAME)



IT **157863-48-4**, 6-Carboxy-4-phenylmethylamino-2-(1-imidazolyl)-5,6,7,8-tetrahydroquinazoline dihydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of aminoquinazolines for use in inhibiting neoplastic cells and related conditions)

RN 157863-48-4 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:553569 CAPLUS
DOCUMENT NUMBER: 133:150575
TITLE: Preparation of substituted 4-amino-2-aryltetrahydroquinazolines as activators of soluble guanylate cyclase
INVENTOR(S): Schindler, Ursula; Schonafinger, Karl; Strobel, Hartmut
PATENT ASSIGNEE(S): Aventis Pharma Deutschland G.m.b.H., Germany
SOURCE: PCT Int. Appl., 42 pp.
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000046214	A1	20000810	WO 2000-EP468	20000122
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19904710	A1	20000810	DE 1999-19904710	19990205
CA 2362363	AA	20000810	CA 2000-2362363	20000122
EP 1150963	A1	20011107	EP 2000-901586	20000122
EP 1150963	B1	20031203		
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JP 2002536369	T2	20021029	JP 2000-597284	20000122
AT 255565	E	20031215	AT 2000-901586	20000122
PT 1150963	T	20040430	PT 2000-901586	20000122
ES 2211503	T3	20040716	ES 2000-901586	20000122
US 6660746	B1	20031209	US 2000-497723	20000204
US 2004063690	A1	20040401	US 2003-674350	20031001
PRIORITY APPLN. INFO.:			DE 1999-19904710 A	19990205
			WO 2000-EP468 W	20000122
			US 2000-497723 A3	20000204

OTHER SOURCE(S): MARPAT 133:150575
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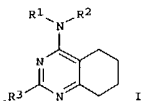

I

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
AB The title compds. [I; R1, R2 = H, (un)substituted alkyl, cycloalkyl, etc.; NR1R2 = (un)substituted 5-7 membered saturated heterocyclyl which can contain one further hetero atom selected from O, S, SO, SO2; R3 = aryl, but cannot be unsubstituted Ph] and their salts which have the ability to modulate the endogenous production of cyclic guanosine monophosphate (cGMP) and are generally suitable for the therapy and prophylaxis of disease states which are associated with a disturbed cGMP balance, for example, cardiovascular disorders such as high blood pressure, angina pectoris, cardiac insufficiency, thromboses or atherosclerosis, were prepared Thus, reacting 2-(4-chlorophenyl)-4-chloro-5,6,7,8-tetrahydroquinazoline (preparation given) with trans-4-aminocyclohexanol hydrochloride in the presence of tert-BuOK and N-methylpyrrolidine afforded (trans)-I.MeSO3H [R1 = trans-4-hydroxycyclohexylamino; R2 = H; R3 = 4-ClC6H4] which showed 28-fold stimulation of the sGC activity at 50 μM.
IT **287472-74-6P 287472-75-7P 287472-76-8P**
287472-77-9P 287472-78-0P 287472-81-5P
287472-83-7P 287472-84-8P 287472-85-9P
287472-86-0P 287472-87-1P 287472-88-2P
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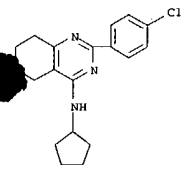
287473-44-3P 287473-45-4P 287473-46-5P
287473-47-6P 287473-48-7P 287473-49-8P
287473-51-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted 4-amino-2-aryltetrahydroquinazolines as activators of soluble guanylate cyclase)

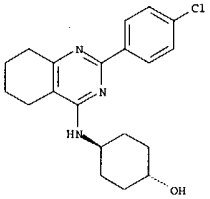
RN 287472-74-6 CAPLUS
CN 4-Quinazolinamine, 2-(4-chlorophenyl)-N-cyclopentyl-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 287472-75-7 CAPLUS
CN Cyclohexanol, 4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



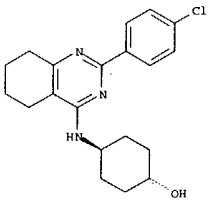
RN 287472-76-8 CAPLUS
CN Cyclohexanol, 4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 287472-75-7
CMF C20 H24 Cl N3 O

Relative stereochemistry.

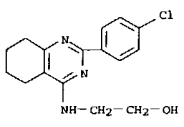
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



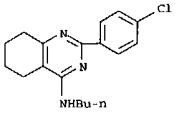
CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 287472-77-9 CAPLUS
CN Ethanol, 2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

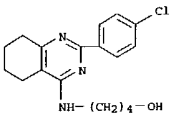


RN 287472-78-0 CAPLUS
CN 4-Quinazolinamine, N-butyl-2-(4-chlorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

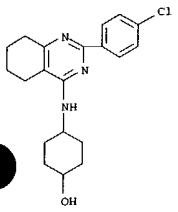


L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 287472-81-5 CAPLUS
CN 1-Butanol, 4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

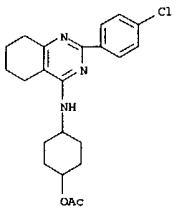


RN 287472-83-7 CAPLUS
CN Cyclohexanol, 4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



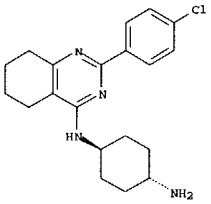
RN 287472-84-8 CAPLUS
CN Cyclohexanol, 4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, acetate (ester) (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287472-85-9 CAPLUS
CN 1,4-Cyclohexanediamine, N-[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]-, trans- (9CI) (CA INDEX NAME)

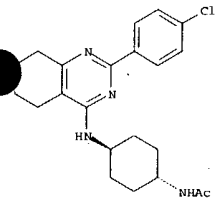
Relative stereochemistry.



RN 287472-86-0 CAPLUS
CN Acetamide, N-[trans-4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

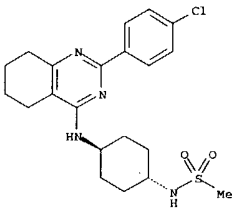
Relative stereochemistry.

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287472-87-1 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

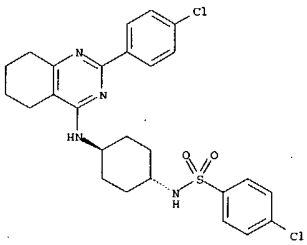
Relative stereochemistry.



RN 287472-88-2 CAPLUS
CN Benzenesulfonamide, 4-chloro-N-[trans-4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

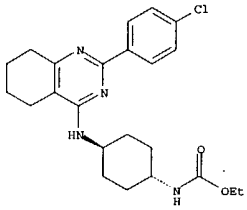
Relative stereochemistry.

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287472-89-3 CAPLUS
CN Carbamic acid, [trans-4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]cyclohexyl]-, ethyl ester (9CI) (CA INDEX NAME)

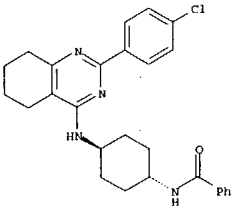
Relative stereochemistry.



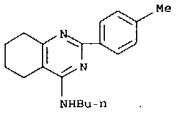
RN 287472-90-6 CAPLUS
CN Benzamide, N-[trans-4-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

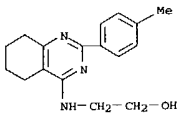
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287472-92-8 CAPLUS
CN 4-Quinazolinamine, N-butyl-5,6,7,8-tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



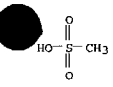
RN 287472-95-1 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(4-methylphenyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



RN 287472-98-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methylphenyl)-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

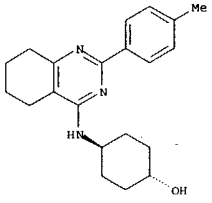
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CRN 75-75-2
CMF C H4 O3 S

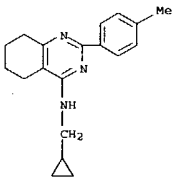


RN 287473-03-4 CAPLUS
CN Cyclohexanol, 4-[[5,6,7,8-tetrahydro-2-(4-methylphenyl)-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

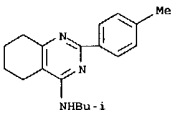


RN 287473-04-5 CAPLUS
CN 4-Quinazolinamine, N-(cyclopropylmethyl)-5,6,7,8-tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)

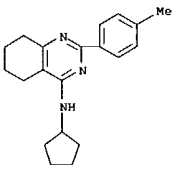


RN 287473-05-6 CAPLUS
CN 4-Quinazolinamine, N-cyclobutyl-5,6,7,8-tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



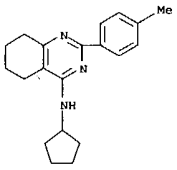
RN 287472-99-5 CAPLUS
CN 4-Quinazolinamine, N-cyclopentyl-5,6,7,8-tetrahydro-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



RN 287473-01-2 CAPLUS
CN 4-Quinazolinamine, N-cyclopentyl-5,6,7,8-tetrahydro-2-(4-methylphenyl)-, monomethanesulfonate (9CI) (CA INDEX NAME)

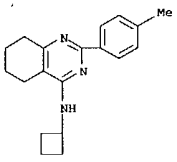
CM 1

CRN 287472-99-5
CMF C20 H25 N3

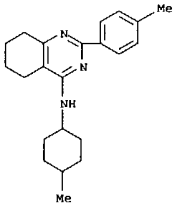


CM 2

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

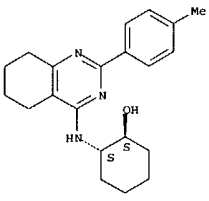


RN 287473-06-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(4-methylcyclohexyl)-2-(4-methylphenyl)- (9CI) (CA INDEX NAME)



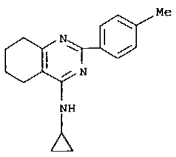
RN 287473-08-9 CAPLUS
CN Cyclohexanol, 2-[[5,6,7,8-tetrahydro-2-(4-methylphenyl)-4-quinazolinyl]amino]-, (1R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

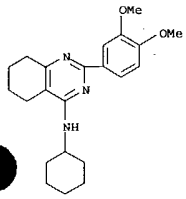


RN 287473-11-4 CAPLUS
CN 4-Quinazolinamine, N-cyclopropyl-5,6,7,8-tetrahydro-2-(4-methylphenyl)-

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

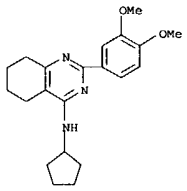


RN 287473-12-5 CAPLUS
CN 4-Quinazolinamine, N-cyclohexyl-2-(3,4-dimethoxyphenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 287473-13-6 CAPLUS
CN 4-Quinazolinamine, N-cyclopentyl-2-(3,4-dimethoxyphenyl)-5,6,7,8-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)

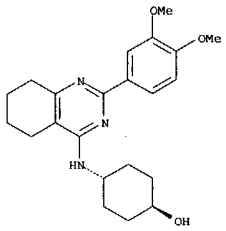
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● HCl

RN 287473-14-7 CAPLUS
CN Cyclohexanol, 4-[[2-(3,4-dimethoxyphenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

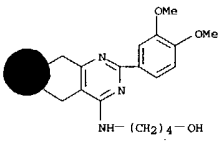
Relative stereochemistry.



● HCl

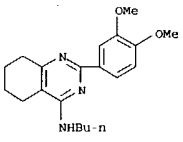
RN 287473-16-9 CAPLUS
CN 1-Butanol, 4-[[2-(3,4-dimethoxyphenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



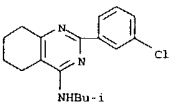
● HCl

RN 287473-17-0 CAPLUS
CN 4-Quinazolinamine, N-butyl-2-(3,4-dimethoxyphenyl)-5,6,7,8-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



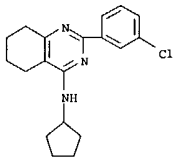
● HCl

RN 287473-20-5 CAPLUS
CN 4-Quinazolinamine, 2-(3-chlorophenyl)-5,6,7,8-tetrahydro-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

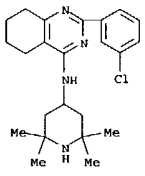


RN 287473-21-6 CAPLUS
CN 4-Quinazolinamine, 2-(3-chlorophenyl)-N-cyclopentyl-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

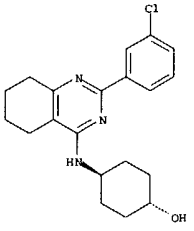


RN 287473-22-7 CAPLUS
CN 4-Quinazolinamine, 2-(3-chlorophenyl)-5,6,7,8-tetrahydro-N-(2,2,6,6-tetramethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)



RN 287473-24-9 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



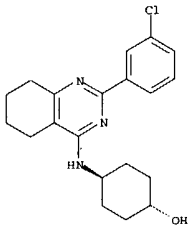
RN 287473-25-0 CAPLUS
CN Cyclohexanol, 4-[[2-(3-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans-, monomethanesulfonate (salt) (9CI) (CA INDEX

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
NAME)

CM 1

CRN 287473-24-9
CMF C20 H24 Cl N3 O

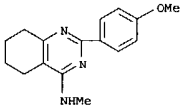
Relative stereochemistry.



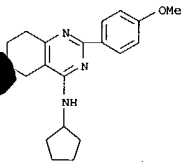
CM 2

CRN 75-75-2
CMF C H4 O3 S

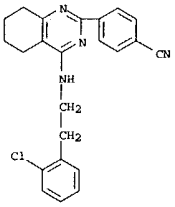
RN 287473-26-1 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methoxyphenyl)-N-methyl- (9CI) (CA INDEX NAME)



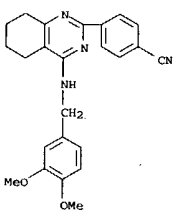
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287473-32-9 CAPLUS
CN Benzonitrile, 4-[4-[[2-(2-chlorophenyl)ethyl]amino]-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)

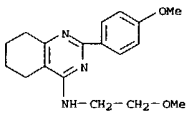


RN 287473-33-0 CAPLUS
CN Benzonitrile, 4-[4-[[(3,4-dimethoxyphenyl)methyl]amino]-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)

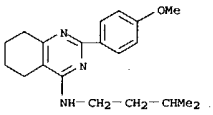


RN 287473-34-1 CAPLUS

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 287473-27-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-(2-methoxyethyl)-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

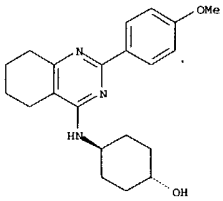


RN 287473-28-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methoxyphenyl)-N-(3-methylbutyl)- (9CI) (CA INDEX NAME)



RN 287473-29-4 CAPLUS
CN Cyclohexanol, 4-[[5,6,7,8-tetrahydro-2-(4-methoxyphenyl)-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

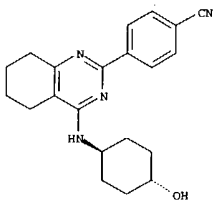
Relative stereochemistry.



RN 287473-30-7 CAPLUS
CN 4-Quinazolinamine, N-cyclopentyl-5,6,7,8-tetrahydro-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

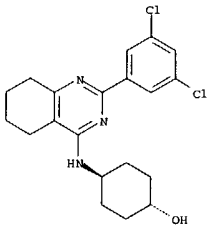
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Benzonitrile, 4-[5,6,7,8-tetrahydro-4-[(trans-4-hydroxycyclohexyl)amino]-2-quinazolinyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



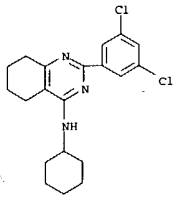
RN 287473-35-2 CAPLUS
CN Cyclohexanol, 4-[[2-(3,5-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

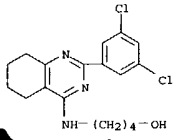


RN 287473-36-3 CAPLUS
CN 4-Quinazolinamine, N-cyclohexyl-2-(3,5-dichlorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



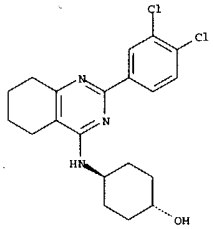
RN 287473-38-5 CAPLUS
CN 1-Butanol, 4-[[2-(3,5-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



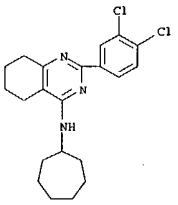
RN 287473-39-6 CAPLUS
CN Cyclohexanol, 4-[[2-(3,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

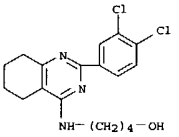
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 287473-40-9 CAPLUS
CN 4-Quinazolinamine, N-cycloheptyl-2-(3,4-dichlorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

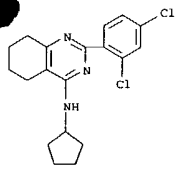


RN 287473-41-0 CAPLUS
CN 1-Butanol, 4-[[2-(3,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



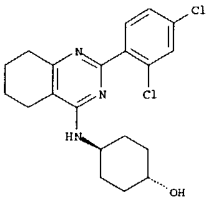
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 287473-42-1 CAPLUS
CN 4-Quinazolinamine, N-cyclopentyl-2-(2,4-dichlorophenyl)-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

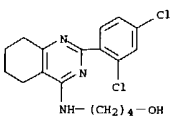


RN 287473-43-2 CAPLUS
CN Cyclohexanol, 4-[[2-(2,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



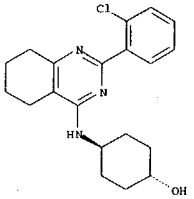
RN 287473-44-3 CAPLUS
CN 1-Butanol, 4-[[2-(2,4-dichlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



RN 287473-45-4 CAPLUS
CN Cyclohexanol, 4-[[2-(2-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

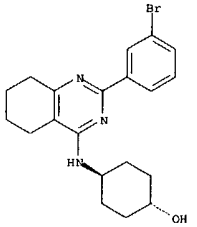
L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Relative stereochemistry.

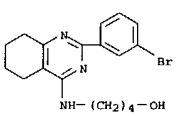


RN 287473-46-5 CAPLUS
CN Cyclohexanol, 4-[[2-(3-bromophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

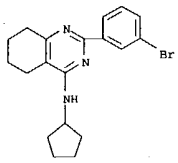


RN 287473-47-6 CAPLUS
CN 1-Butanol, 4-[[2-(3-bromophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



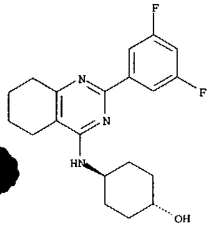
RN 287473-48-7 CAPLUS
CN 4-Quinazolinamine, 2-(3-bromophenyl)-N-cyclopentyl-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



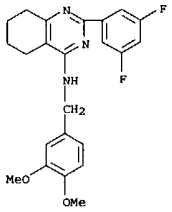
RN 287473-49-8 CAPLUS
CN Cyclohexanol, 4-[[2-(3,5-difluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 287473-51-2 CAPLUS
CN 4-Quinazolinamine, 2-(3,5-difluorophenyl)-N-[(3,4-dimethoxyphenyl)methyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)

L3 ANSWER 15 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



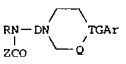
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:407087 CAPLUS
DOCUMENT NUMBER: 131:97602
TITLE: Condensed heterocyclic compounds as 5-HT2 receptor antagonists and pharmaceuticals containing them
INVENTOR(S): Kuroita, Takanobu; Bogauchi, Masahiro; Fujio, Masakazu; Nakagawa, Haruto
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 72 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11171865	A2	19990629	JP 1997-334675	19971204
PRIORITY APPLN. INFO.:			JP 1997-334675	19971204

OTHER SOURCE(S): MARPAT 131:97602
GI



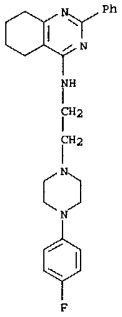
I

AB Pharmaceutical compns., e.g. blood platelet aggregation inhibitor, pharmaceuticals for improvement of peripheral circulation, etc., contain title compds. I [R = condensed N-containing heterocyclyl; Z = C1-8 (cyclo)alkyl, (substituted) Ph or heteroaryl; D = C1-8 alkylene; QT = CH, CH2N, (CH2)2N, CH2CH, CH:C; G = none, C1-8 alkylene, CO, CH(OH); Ar = (substituted) (hetero)aryl, condensed heteroaryl], their optical isomers, or their salts as 5-HT2 receptor antagonists. N-(4,5,6,7-tetrahydro-2-methyl-2H-indazol-3-yl)benzamide (1.0 g; preparation given) was treated with NaH in DMF in the presence of NaI at room temperature for 30 min and condensed with 1.0 g 4-benzoyl-1-(2-chloroethyl)piperidine at 70° to give 0.4 g I (R = 4,5,6,7-tetrahydro-2-methyl-2H-indazol-3-yl, Z = Ar = Ph, D = (CH2)2, QT = CH2CH, G = CO), which in vitro showed 5-HT-induced blood platelet aggregation inhibition with IC50 of 0.026 μM, vs. 0.26 μM, for sarpogrelate.

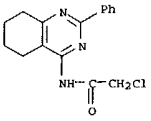
IT **200412-44-8P 200413-54-3P 231283-51-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of condensed heterocyclic compds. as 5-HT2 receptor antagonists)

RN 200412-44-8 CAPLUS
CN 4-Quinazolinamine, N-[2-[4-(4-fluorophenyl)-1-piperazinyl]ethyl]-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

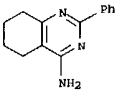
L3 ANSWER 16 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 200413-54-3 CAPLUS
CN Acetamide, 2-chloro-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)



RN 231283-51-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

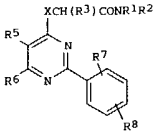


10/ 674,350

L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:314282 CAPLUS
DOCUMENT NUMBER: 129:54385
TITLE: Preparation of acetic acid amide derivatives as drugs
INVENTOR(S): Murata, Akiya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Ito, Mari
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10130150	A2	19980519	JP 1997-257573	19970905
PRIORITY APPLN. INFO.:			JP 1996-257704	19960905

OTHER SOURCE(S): MARPAT 129:54385
GI

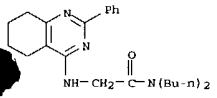


I

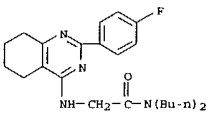
AB The title compds. [I; X = O, NR4; R1 = H, (un)substituted lower alkyl or alkenyl, etc.; R2 = cycloalkyl, lower alkyl, (un)substituted Ph, etc.; R3 = H, alkyl, hydroxyalkyl, etc.; R4 = H, alkyl, or combine with R3 and N to form a pyrrolidine or piperidine; R5 = H, lower alkyl or alkenyl, hydroxyalkyl, CF3, etc.; R6 = H, lower alkyl, CF3, etc.; R7 = H, halo, lower alkyl, etc.; R8 = H, halo, lower alkoxy, etc.] are prepared I, possessing affinity toward the benzodiazepine receptor, are useful for prevention and treatment of melancholia, insecure related diseases, central nervous system diseases, and immunity inflammation diseases. Thus, 4-chloro-5,6-dimethyl-2-phenylpyrimidine was reacted with 2-amino-N,N-dipropylacetamide in the presence of Et3N to give I (R1 = R2 = n-Pr, R3 = R7 = R8 = H, R5 = R6 = Me, X = NH), which showed IC50 of 3.10 nM with abenzodiazepine receptor (BZ@3) when tested with rat. A formulation containing I was also prepared

IT **184108-67-6P 184108-68-7P 184108-69-8P**
184108-70-1P 184108-71-2P 184108-72-3P
184108-73-4P 184108-74-5P 184108-78-9P
184108-79-0P 184108-80-3P 184108-81-4P
184108-82-5P 184108-83-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acetic acid amide derivs. as drugs)

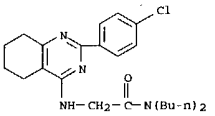
L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 184108-71-2 CAPLUS
CN Acetamide, N,N-dibutyl-2-[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



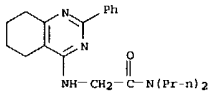
RN 184108-72-3 CAPLUS
CN Acetamide, N,N-dibutyl-2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)



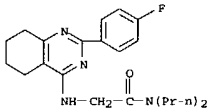
RN 184108-73-4 CAPLUS
CN Acetamide, N-(4-chlorophenyl)-N-methyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 184108-67-6 CAPLUS
CN Acetamide, N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)



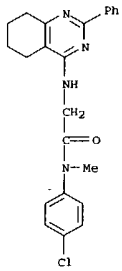
RN 184108-68-7 CAPLUS
CN Acetamide, 2-[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)



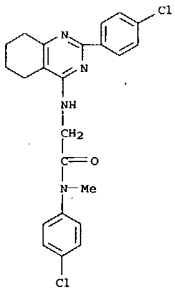
RN 184108-69-8 CAPLUS
CN Acetamide, 2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

RN 184108-70-1 CAPLUS
CN Acetamide, N,N-dibutyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

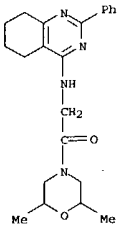


RN 184108-74-5 CAPLUS
CN Acetamide, N-(4-chlorophenyl)-2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

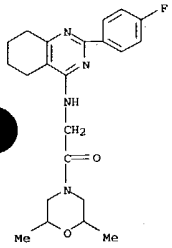


RN 184108-78-9 CAPLUS
CN Morpholine, 2,6-dimethyl-4-[[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]acetyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

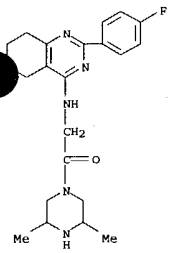


RN 184108-79-0 CAPLUS
CN Morpholine, 4-[[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-2,6-dimethyl- (9CI) (CA INDEX NAME)

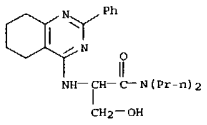


RN 184108-80-3 CAPLUS
CN Morpholine, 4-[[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-2,6-dimethyl- (9CI) (CA INDEX NAME)

L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

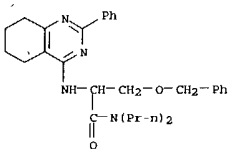


RN 184108-83-6 CAPLUS
CN Propanamide, 3-hydroxy-N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

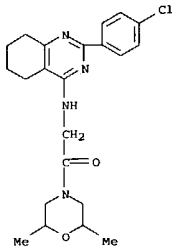


IT **184110-07-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acetic acid amide derivs. as drugs)

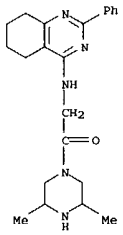
RN 184110-07-4 CAPLUS
CN Propanamide, 3-(phenylmethoxy)-N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 17 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 184108-81-4 CAPLUS
CN Piperazine, 3,5-dimethyl-1-[[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]acetyl]- (9CI) (CA INDEX NAME)



RN 184108-82-5 CAPLUS
CN Piperazine, 1-[[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

L3 ANSWER 18 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:226895 CAPLUS
DOCUMENT NUMBER: 128:304069
TITLE: Inhibitors for nitric oxide formation
INVENTOR(S): Taniguchi, Naoyuki; Nakai, Hisao
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

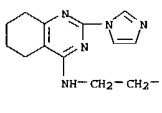
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10087492	A2	19980407	JP 1997-183227	19970625

PRIORITY APPLN. INFO.: JP 1996-164593 19960625

AB Imidazolyl quinazoline, aminopyrimidine, and pyrimidine derivs. (Markush included) and their salts are claimed as inhibitors for nitric oxide formation for prevention and treatment of related diseases e.g. shock, hypotension, chronic rheumatism, ulcerative colitis, brain ischemia, tumor, insulin-dependent diabetes, etc. Examples of pharmaceutical tablets and injections were formulated.

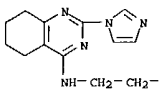
IT **157863-56-4 184673-90-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors for nitric oxide formation for treatment of related diseases)

RN 157863-56-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 184673-90-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



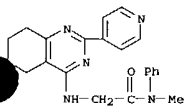
L3 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:175920 CAPLUS
DOCUMENT NUMBER: 128:230383
TITLE: Preparation and formulation of pyrimidine derivatives as pharmaceuticals with affinity for peripheral benzodiazepine receptors
INVENTOR(S): Murata, Teruya; Kondo, Katsunori; Furukawa, Kiyoshi; Oka, Makoto
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9809960	A1	19980312	WO 1997-JP3079	19970903
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9707427	A	19980302	ZA 1997-7427	19970819
AU 9741342	A1	19980326	AU 1997-41342	19970903
PRIORITY APPLN. INFO.:			JP 1996-255420 A	19960904
			WO 1997-JP3079 W	19970903

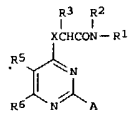
OTHER SOURCE(S): MARPAT 128:230383
GI

L3 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

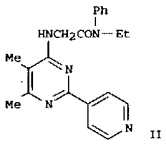


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



I



II

AB The title compds. I [X represents O or NR4; R1 represents H, lower alkyl, etc.; R2 represents lower alkyl, lower alkenyl, etc.; R3 represents H, lower alkyl, etc.; R4 represents H or lower alkyl; R5 represents H, lower alkyl, etc. or halogeno, hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, etc.; R6 represents H, lower alkyl, etc. or hydroxy(lower)alkyl, lower alkoxy(lower)alkyl, etc., or R5 and R6 may form together (CH2)n (wherein n is 3 to 6); and A represents optionally substituted heteroaryl or optionally substituted Ph] are prepared These compds. are expected to be useful as remedies and preventives for central diseases, for example, diseases associated with anxiety, such as neurosis and psychosomatic disorder, depression and epilepsy; circulatory diseases such as angina pectoris and hypertension; immunol. nervous diseases such as multiple sclerosis; or immunol. inflammatory diseases such as rheumatism. In an in vitro test for affinity for the peripheral benzodiazepine receptors, the title compound II showed IC50 of 0.25 nM.

IT **204393-43-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as pharmaceuticals with affinity for peripheral benzodiazepine receptors)

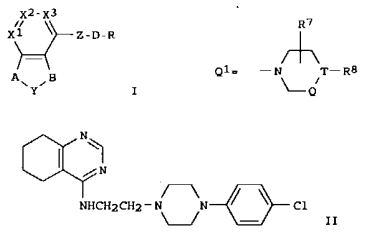
RN 204393-43-1 CAPLUS
CN Acetamide, N-methyl-N-phenyl-2-[[5,6,7,8-tetrahydro-2-(4-pyridinyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:13943 CAPLUS
DOCUMENT NUMBER: 128:61522
TITLE: Preparation of fused heterocyclic compounds as antagonists of D2 and D4 receptors
INVENTOR(S): Kuroita, Takanobu; Togo, Yoshifumi; Ishibuchi, Seigo; Fujio, Masakazu; Futamura, Takashi
PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 176 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9747601	A1	19971218	WO 1997-JP1993	19970609
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9729807	A1	19980107	AU 1997-29807	19970609
JP 3531169	B2	20040524	JP 1998-501435	19970609
PRIORITY APPLN. INFO.:			JP 1996-149620 A	19960611
			WO 1997-JP1993 W	19970609

OTHER SOURCE(S): MARPAT 128:61522
GI



I

II

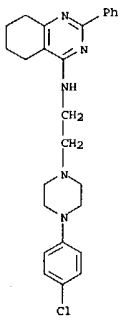
AB Fused heterocyclic compds. represented by general formula [I; X1-X2-X3 = NCR1N, CR1CR2N, NCR1CR2, CR1NCR2, NNCR1; R1, R2 = H, alkyl, OH, NH2, arylalkyl, (un)substituted aryl or heteroaryl; A = linear or branched and (un)substituted C1-4 alkyl; Y = O, S, SO, SO2, (un)substituted NH; B = linear or branched alkyl and (un)substituted C1-4 alkylene; Z = O, S, SO, SO2, (un)substituted NH, CH(OH), CO, CH2; D = linear or branched alkyl

L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
C1-8 alkylene; R = heterocyclyl, e.g., Q1; wherein Q-T = (CH2)n, CH2CH, CH:C; wherein R7 = H, alkyl; R8 = (un)substituted arom. hydrocarbyl or heterocyclyl] or optical isomers or pharmaceutically acceptable salts thereof are prepd. Also claimed are medicinal compns. comprising these compds. and pharmaceutically acceptable additives, and drugs comprising these compds. These compds. exert more potent blocking effects on D4 receptors than on D2 receptors. Moreover, they have high affinities for receptors other than dopamine receptors such as muscarine M1, and serotonin-2 (5-HT2) and adrenalin.α1 and α2 receptors. Thus, these compds. are efficacious against not only pos. symptoms typified by hallucination and delusion characteristic of the acute stage of schizophrenia but also neg. symptoms such as emotional torpidity, abulia, and autism. In addn., they are useful as antipsychotic agents with relieved side effects such as extrapyramidal symptoms and abnormal internal secretion obsd. in assocn. with the administration of the conventional antipsychotic agents having only D2 receptor antagonism. The above compds. are usable as remedies for diseases such as schizophrenia. Thus, N-(5,6,7,8-tetrahydroquinazolin-4-yl)-2-chloroacetamide (prepn. given) and N-(4-chlorophenyl)piperazine hydrochloride were dissolved in DMF and stirred with K2CO3 and KI at room temp. for 24 h to give N-(5,6,7,8-tetrahydroquinazolin-4-yl)-2-[4-(4-chlorophenyl)piperazin-1-yl]acetamide, which was reduced by LiAlH4 in THF at room temp. for 30 min to give the title compd. (II). II and another compd. tested in vitro showed affinity for D2 and D4 receptors of nerve synapses membrane with Ki value of ≥5 nM and 0.01-1 nM, resp.

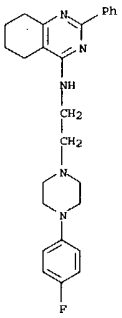
IT **200412-43-7P 200412-44-8P 200412-46-0P**
200412-48-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused heterocyclic compds. having antagonism for D2 and D4 receptors as antipsychotics)

RN 200412-43-7 CAPLUS
CN 4-Quinazolinamine, N-[2-[4-(4-chlorophenyl)-1-piperazinyl]ethyl]-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 200412-44-8 CAPLUS
CN 4-Quinazolinamine, N-[2-[4-(4-fluorophenyl)-1-piperazinyl]ethyl]-5,6,7,8-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

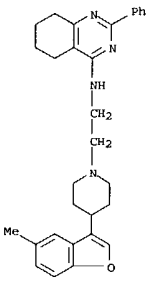


RN 200412-46-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-[2-[4-(5-methyl-3-benzofuranyl)-1-

L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
piperidinyl]ethyl]-2-phenyl-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

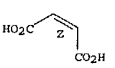
CRN 200412-45-9
CMF C30 H34 N4 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

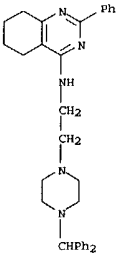


RN 200412-48-2 CAPLUS
CN 4-Quinazolinamine, N-[2-[4-(diphenylmethyl)-1-piperazinyl]ethyl]-5,6,7,8-tetrahydro-2-phenyl-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 200412-47-1
CMF C33 H37 N5

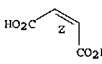
L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



CM 2

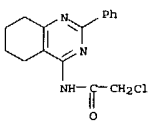
CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.



IT **200413-54-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of fused heterocyclic compds. having antagonism for D2 and D4 receptors as antipsychotics)

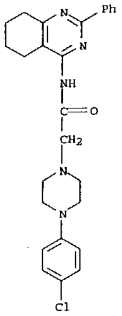
RN 200413-54-3 CAPLUS
CN Acetamide, 2-chloro-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)



IT **200413-45-2P 200413-46-3P 200413-47-4P**
200413-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of fused heterocyclic compds. having antagonism for D2 and D4 receptors as antipsychotics)

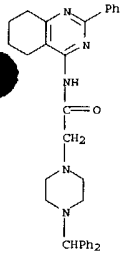
10/ 674,350

L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 200413-45-2 CAPLUS
CN 1-Piperazineacetamide, 4-(4-chlorophenyl)-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)

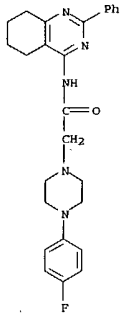


RN 200413-46-3 CAPLUS
CN 1-Piperazineacetamide, 4-(4-fluorophenyl)-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)

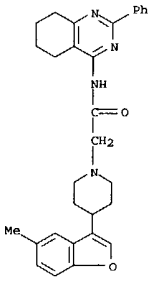
L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L3 ANSWER 20 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 200413-47-4 CAPLUS
CN 1-Piperidineacetamide, 4-(5-methyl-3-benzofuranyl)-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)



RN 200413-48-5 CAPLUS
CN 1-Piperazineacetamide, 4-(diphenylmethyl)-N-(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)- (9CI) (CA INDEX NAME)

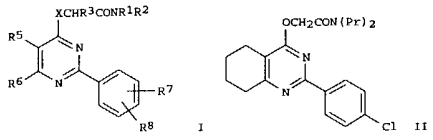
L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:753799 CAPLUS
DOCUMENT NUMBER: 126:18884
TITLE: Preparation and formulation of pyrimidine derivatives as agents with effect on the peripheral benzodiazepine receptors
INVENTOR(S): Murata, Teruya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Itoh, Mari
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9632383	A1	19961017	WO 1996-JP977	19960410
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML				
IL 117659	A1	20001206	IL 1996-117659	19960326
ZA 9602438	A	19961001	ZA 1996-2438	19960327
CA 2218033	AA	19961017	CA 1996-2218033	19960410
AU 9652874	A1	19961030	AU 1996-52874	19960410
AU 694647	B2	19980723		
EP 826673	A1	19980304	EP 1996-909327	19960410
EP 826673	B1	20021120		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1186487	A	19980701	CN 1996-194408	19960410
CN 1094929	B	20021127		
BR 9604894	A	19980714	BR 1996-4894	19960410
RU 2160256	C2	20001210	RU 1997-118591	19960410
SK 281840	B6	20010806	SK 1997-1374	19960410
CZ 289093	B6	20011017	CZ 1997-3223	19960410
RO 117532	B1	20020430	RO 1997-1858	19960410
AT 228113	E	20021215	AT 1996-909327	19960410
PT 826673	T	20030228	PT 1996-909327	19960410
ES 2187644	T3	20030616	ES 1996-909327	19960410
TW 450963	B	20010821	TW 1996-85104372	19960412
NO 9704685	A	19971212	NO 1997-4685	19971010
US 5972946	A	19991026	US 1997-930604	19971014
PRIORITY APPLN. INFO.:			JP 1995-113937 A	19950413
			WO 1996-JP977 W	19960410

OTHER SOURCE(S): MARPAT 126:18884
GI

L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



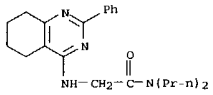
I

II

AB The title compds. I [X represents O or NR4; R1 represents H, lower alkyl, lower alkenyl or cycloalkyl(lower)alkyl; R2 represents lower alkyl, cycloalkyl, optionally substituted Ph, etc.; R3 represents H, lower alkyl or hydroxy(lower)alkyl; R4 represents H, lower alkyl, etc.; R5 represents hydroxy(lower)alkyl, etc.; R6 represents H, lower alkyl, CF3 or optionally substituted Ph, or R5 and R6 together form (CH2)n; n = 3 - 6; R7 represents H, halogeno, lower alkyl, lower alkoxy, CF3, OH, NH2, etc.; and R8 represents H, halogeno, lower alkyl or lower alkoxyl are prepared In an in vitro test for affinity for the peripheral benzodiazepine receptors, the title compound II in vitro showed IC50 of 0.89 nM.

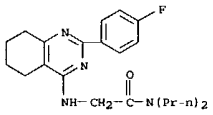
IT **184108-67-6P 184108-68-7P 184108-69-8P**
184108-70-1P 184108-71-2P 184108-72-3P
184108-73-4P 184108-74-5P 184108-78-9P
184108-79-0P 184108-80-3P 184108-81-4P
184108-82-5P 184108-83-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as agents with effect on peripheral benzodiazepine receptors)

RN 184108-67-6 CAPLUS
CN Acetamide, N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

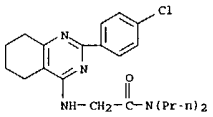


RN 184108-68-7 CAPLUS
CN Acetamide, 2-[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)

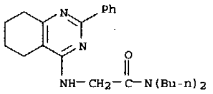
L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



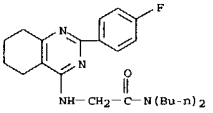
RN 184108-69-8 CAPLUS
CN Acetamide, 2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N,N-dipropyl- (9CI) (CA INDEX NAME)



RN 184108-70-1 CAPLUS
CN Acetamide, N,N-dibutyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

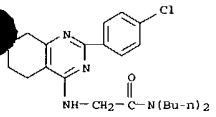


RN 184108-71-2 CAPLUS
CN Acetamide, N,N-dibutyl-2-[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

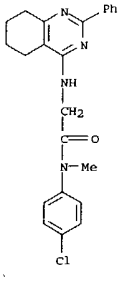


RN 184108-72-3 CAPLUS

L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Acetamide, N,N-dibutyl-2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

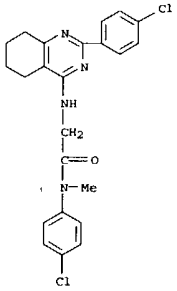


RN 184108-73-4 CAPLUS
CN Acetamide, N-(4-chlorophenyl)-N-methyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

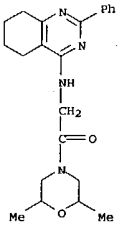


RN 184108-74-5 CAPLUS
CN Acetamide, N-(4-chlorophenyl)-2-[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

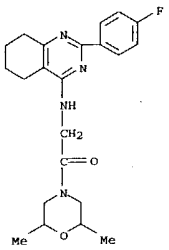


RN 184108-78-9 CAPLUS
CN Morpholine, 2,6-dimethyl-4-[[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]acetyl]- (9CI) (CA INDEX NAME)

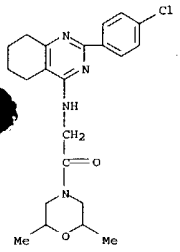


RN 184108-79-0 CAPLUS
CN Morpholine, 4-[[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-2,6-dimethyl- (9CI) (CA INDEX NAME)

L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

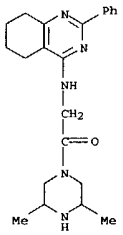


RN 184108-80-3 CAPLUS
CN Morpholine, 4-[[[2-(4-chlorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-2,6-dimethyl- (9CI) (CA INDEX NAME)

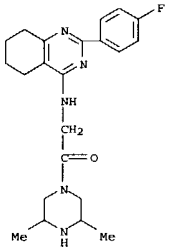


RN 184108-81-4 CAPLUS
CN Piperazine, 3,5-dimethyl-1-[[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]acetyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

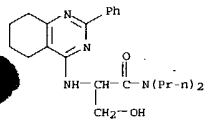


RN 184108-82-5 CAPLUS
CN Piperazine, 1-[[[2-(4-fluorophenyl)-5,6,7,8-tetrahydro-4-quinazolinyl]amino]acetyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

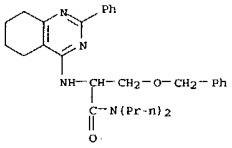


RN 184108-83-6 CAPLUS
CN Propanamide, 3-hydroxy-N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)

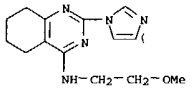
L3 ANSWER 21 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **184110-07-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidine derivs. as agents with effect on peripheral benzodiazepine receptors)
RN 184110-07-4 CAPLUS
CN Propanamide, 3-(phenylmethoxy)-N,N-dipropyl-2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (9CI) (CA INDEX NAME)



L3 ANSWER 22 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:675493 CAPLUS
DOCUMENT NUMBER: 126:26533
TITLE: Quinazoline derivatives suppress nitric oxide production by macrophages through inhibition of NOS II gene expression
AUTHOR(S): Fujiwara, Noriko; Okado, Ayako; Seo, Han Geuk; Fujii, Junichi; Kondo, Kigen; Taniguchi, Naoyuki
CORPORATE SOURCE: Department Biochemistry, Osaka University Medical School, Suita, 565, Japan
SOURCE: FEBS Letters (1996), 395(2,3), 299-303
CODEN: FEBLAL; ISSN: 0014-5793
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have found three novel quinazolidine derivs. which inhibit the formation of nitrite dose-dependently in a murine macrophage cell line, RAW264.7. The decreased nitrite formation was due not to the inhibition of nitric oxide synthase activity but to suppression of NOS II mRNA and protein expression. In rat vascular smooth muscle cells (VSMC), however, these compound rather enhanced NOS II mRNA. These compds. also prevented LPS-stimulated heme oxygenase-1 (HO-1) and cyclooxygenase-2 (COx-2) gene expression in RAW264.7 cells, but again not in VSMC. The three quinazolidine derivs. specifically inhibit gene expression of NOS II, HO-1 and COX-2 only in macrophage cells, indicating that they are selective inhibitors of inducible gene expression in macrophages.
IT **184673-90-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(quinazoline derivs. suppress nitric oxide production by macrophages through inhibition of NOS II gene expression)
RN 184673-90-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)- (9CI) (CA INDEX NAME)



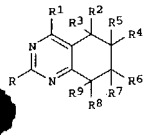
same as other references

L3 ANSWER 23 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:483914 CAPLUS
DOCUMENT NUMBER: 125:135459
TITLE: Preparation of insecticidal substituted-2,4-diamino-5,6,7,8-tetrahydroquinazolines
INVENTOR(S): Cullen, Thomas G.; Henrie, Ii Robert N.; Peake, Clinton J.; Bennett, Brian D.
PATENT ASSIGNEE(S): FMC Corp., USA
SOURCE: U.S., 31 pp., Cont. of U.S. Ser. No. 111,802, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

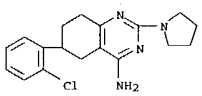
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5536725	A	19960716	US 1994-319504	19941006
US 5712281	A	19980127	US 1995-445201	19950523
PRIORITY APPLN. INFO.:			US 1993-111802	19930825
			US 1994-319504	19941006

OTHER SOURCE(S): MARPAT 125:135459
GI



I

AB The title compds. I [R = (un)substituted amino, pyrrolidin-1-yl, piperidin-1-yl, etc.; R1 = amino; R2,R6 = H, alkyl; R3,R5,R7 R8,R9 = H; R4 = H, alkyl,CMe3, (un)substituted Ph, etc.] are prepared as insecticides.
IT **180005-06-5P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as insecticide)
RN 180005-06-5 CAPLUS
CN 4-Quinazolinamine, 6-(2-chlorophenyl)-5,6,7,8-tetrahydro-2-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



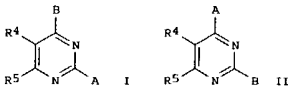
L3 ANSWER 23 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L3 ANSWER 24 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

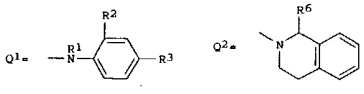
ACCESSION NUMBER: 1996:401560 CAPLUS
DOCUMENT NUMBER: 125:58535
TITLE: Preparation of pyrimidine derivatives as gastric secretion inhibitors
INVENTOR(S): Lee, Jong Wook; Chae, Jeong Seok; Kim, Chang Seop; Kim, Jae Kyu; Lim, Dae Sung; Shon, Moon Kyu; Choi, Yeon Shik; Lee, Sang Ho
PATENT ASSIGNEE(S): Yuhan Corporation, S. Korea
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9605177	A1	19960222	WO 1995-KR105	19950810
W: AU, CA, CN, JP, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
KR 157075	B1	19981116	KR 1994-19997	19940813
KR 157076	B1	19981116	KR 1994-19998	19940813
CA 2197298	AA	19960222	CA 1995-2197298	19950810
AU 9531225	A1	19960307	AU 1995-31225	19950810
AU 688087	B2	19980305		
EP 775120	A1	19970528	EP 1995-927092	19950810
EP 775120	B1	20030604		
R: CH, DE, ES, FR, GB, IT, LI, SE				
CN 1155281	A	19970723	CN 1995-194599	19950810
CN 1102144	B	20030226		
JP 09509188	T2	19970916	JP 1995-507208	19950810
JP 2896532	B2	19990531		
RU 2129549	C1	19990427	RU 1997-104208	19950810
ES 2201112	T3	20040316	ES 1995-927092	19950810
US 5750531	A	19980512	US 1997-776220	19970123
HK 1001618	A1	20030822	HK 1998-100535	19980121
PRIORITY APPLN. INFO.:			KR 1994-19997 A	19940813
			KR 1994-19998 A	19940813
			WO 1995-KR105 W	19950810

OTHER SOURCE(S): MARPAT 125:58535
GI

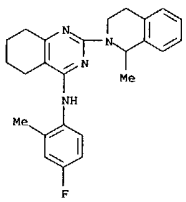


I II



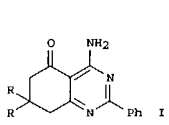
L3 ANSWER 24 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

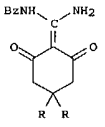
AB The title compds. I and II [R4 and R5, which may be the same or different, are independently hydrogen or a C1-C3 alkyl group, or jointly form a cyclopentyl or cyclohexyl ring; A is Q1 wherein R1 and R2 are, independently of each other, hydrogen or a C1-C3 alkyl group, and R3 is hydrogen, a C1-C3 alkyl group or a halogen; and B is Q2, etc.; R6 is hydrogen or a C1-C3 alkyl group] are prepared 2-(2-Methyl-4-fluorophenylamino)-4-(1-methyl-1,2,3,4-tetrahydroisoquinolin-2-yl)pyrimidine hydrochloride (preparation given) in vitro showed IC50 of 5.4 μM against H+/K+ ATPase, vs. 5.8 μM for omeprazole. The inhibition of enzyme activity by compds. of this invention is reversible.
IT **178308-06-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidine derivs. as gastric secretion inhibitors)
RN 178308-06-0 CAPLUS
CN 4-Quinazolinamine, 2-(3,4-dihydro-1-methyl-2(1H)-isoquinolinyl)-N-(4-fluoro-2-methylphenyl)-5,6,7,8-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



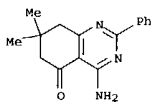
● HCl

L3 ANSWER 25 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:395100 CAPLUS
DOCUMENT NUMBER: 125:167901
TITLE: Chelate synthesis of 4-amino-5,6,7,8-tetrahydroquinazolin-5-one derivatives
AUTHOR(S): Dorokhov, V. A.; Present, M. A.
CORPORATE SOURCE: N.D. Zelinsky Inst. Organic Chem., Russian Acad. Scis., Moscow, 117913, Russia
SOURCE: Izvéstiya Akademii Nauk, Seriya Khimicheskaya (1993), (8), 1504-1505
CODEN: IASKEA
PUBLISHER: Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI


I

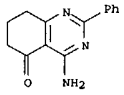

II

AB Title compds. I (R = H, Me) were prepared by reaction of NH3 with the difluoroboron chelates of diaminomethylene diketones II.
IT **43103-05-5P 180059-33-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 43103-05-5 CAPLUS
CN 5(6H)-Quinazolinone, 4-amino-7,8-dihydro-7,7-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 180059-33-0 CAPLUS
CN 5(6H)-Quinazolinone, 4-amino-7,8-dihydro-2-phenyl- (9CI) (CA INDEX NAME)

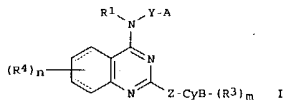
L3 ANSWER 25 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

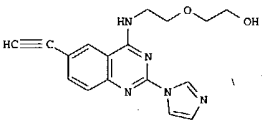


L3 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:795361 CAPLUS
DOCUMENT NUMBER: 124:29779
TITLE: 4-Aminoquinazoline derivatives as inhibitors of cGMP phosphodiesterase and TXA2 synthetase
INVENTOR(S): Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: U.S., 42 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5439895	A	19950808	US 1993-154691	19931119
JP 06192235	A2	19940712	JP 1993-197039	19930714
CA 2100626	AA	19940116	CA 1993-2100626	19930715
AT 208771	E	20011115	AT 1993-305557	19930715
ES 2167325	T3	20020516	ES 1993-305557	19930715
PT 579496	T	20020531	PT 1993-305557	19930715
JP 08099962	A2	19960416	JP 1995-264667	19950920
JP 2923742	B2	19990726		
PRIORITY APPLN. INFO.:			US 1992-913473	B2 19920715
			US 1993-76431	B2 19930614
OTHER SOURCE(S):		MARPAT 124:29779		

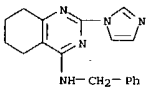
GI


I


II

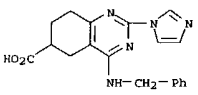
AB The compds. of the formula I and acid addition salts thereof, salts thereof, and hydrates thereof wherein R1 is hydrogen or C1-4 alkyl; Y is C1-6 alkylene; A is OR0 or S(O)pR0, in which R0 is C1-4 alkyl-hydroxy; p is 0-2; Z is single bond, methylene, ethylene, vinylene or ethynylene; CyB is (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing

L3 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially satd., monocyclic hetero ring contg. as hetero atoms, two or three nitrogen atoms, (3) 6-membered, unsatd. or partially satd., monocyclic hetero ring contg. as hetero atom, one nitrogen atom, (4) 4- or 5-membered, unsatd. or partially satd., monocyclic hetero ring contg. as hetero atoms, one, two or three nitrogen atoms, or (5) 4-7 membered, unsatd. or partially satd., monocyclic hetero ring contg. as hetero atoms, one or two oxygen atoms, or one or two sulfur atoms; R3 = e.g., H, C1-4 alkyl, C1-4 alkoxy; R4 = e.g., H, C1-4 alkyl, C1-4 alkoxy; and m and n independently are 1 or 2; with the proviso that (1) a CyB ring does not bond to Z through a nitrogen atom in the CyB ring when Z is vinylene or ethynylene, have inhibitory effect on cGMP-PDE, and addnl. on TXA2 synthetase. Thus, e.g., 2-(1-imidazolyl)-4-[2-(2-hydroxyethoxy)ethyl]amino-6-ethynylquinazoline.2HCl (II.2HCl) (prepd. by desilylation of a silylacetylene precursor) exhibited inhibitory effect on cGMP-PDE and TXA2 synthetase with IC50 = 4.6 + 10-8 M and 1.33 + 10-6 M, resp. Pharmaceutical formulations were given.
IT **157863-44-0P 157863-48-4P 157863-56-4P**
157863-62-2P 157863-78-0P 157863-79-1P
157863-80-4P 157863-88-2P 171661-65-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(4-aminoquinazoline derivs. as inhibitors of cGMP phosphodiesterase and TXA2 synthetase)
RN 157863-44-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(phenylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

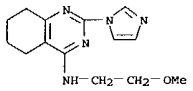
RN 157863-48-4 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

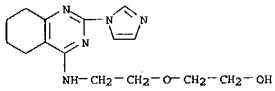
RN 157863-56-4 CAPLUS

L3 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



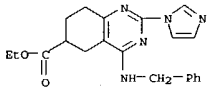
●2 HCl

RN 157863-62-2 CAPLUS
CN Ethanol, 2-[2-[[5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-quinazolinyl]amino]ethoxy]-, dihydrochloride (9CI) (CA INDEX NAME)



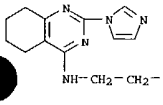
●2 HCl

RN 157863-78-0 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

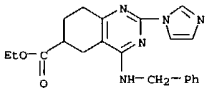


RN 157863-79-1 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

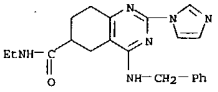


L3 ANSWER 26 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



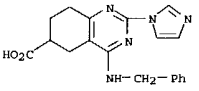
●2 HCl

RN 157863-80-4 CAPLUS
CN 6-Quinazolinecarboxamide, N-ethyl-5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 157863-88-2 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

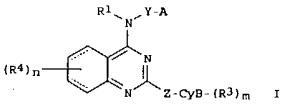
RN 171661-65-7 CAPLUS
CN Ethanol, 2-[2-[[5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-quinazolinyl]amino]ethoxy]- (9CI) (CA INDEX NAME)

L3 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1995:761961 CAPLUS
DOCUMENT NUMBER:	123:340173
TITLE:	4-Aminoquinazoline derivatives as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase
INVENTOR(S):	Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.
PATENT ASSIGNEE(S):	Ono Pharmaceutical Co., Ltd., Japan
SOURCE:	U.S., 44 pp. Cont.-in-part of U.S. Ser. No. 76,431, abandoned. CODEN: USXXAM
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	3
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5436233	A	19950725	US 1993-154518	19931119
JP 06192235	A2	19940712	JP 1993-197039	19930714
CA 2100626	AA	19940116	CA 1993-2100626	19930715
AT 208771	E	20011115	AT 1993-305557	19930715
ES 2167325	T3	20020516	ES 1993-305557	19930715
PT 579496	T	20020531	PT 1993-305557	19930715
JP 08099962	A2	19960416	JP 1995-264667	19950920
JP 2923742	B2	19990726		
PRIORITY APPLN. INFO.:			US 1992-913473	B2 19920715
			US 1993-76431	B2 19930614
OTHER SOURCE(S):	MARPAT 123:340173			

GI

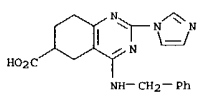


AB Title compds. I [R1 is H, C1-4 alkyl; Y is a single bond or C1-6 alkylene; A is (i) CyA-(R2)l, (ii) OR0 or S(O)pR0 in which R0 is R0A or R0B; R0A is CyA-(R2)l; R0B is H or C1-4 alkyl; p is 0-2; CyA is, e.g., (1) 3-7 membered, saturated or unsatd., monocyclic carbocyclic ring, (2) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
one nitrogen atom, one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms, (3) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,
one nitrogen and one oxygen atoms, two nitrogen and one oxygen atoms, or one nitrogen and two oxygen atoms; R2 is R2A or R2B; R2A is, e.g., CF3, OCF3; R2B is, e.g., H, C1-4 alkyl, C1-4 alkoxy; Z is ZA or ZB, ZA is methylene, ethylene, vinylene, ethynylene; ZB is a single bond; CyB is, e.g., (1) 7-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms, one, two or three nitrogen atoms, (2) 6-membered, unsatd. or partially saturated, monocyclic hetero ring containing as hetero atoms,

L3 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
two or three nitrogen atoms, (3) 6-membered, unsatd. or partially satd., monocyclic hetero ring contg. as a hetero atom, one nitrogen atom; R3 = e.g., H, C1-4 alkyl; R4 = e.g., NHSO2R11, R11 = e.g., C1-4 alkyl; l, m, n are independently 1 or 2 (with provisos)] are provided as inhibitors of cGMP-PDE and TXA2 synthetase. Thus, e.g., treatment of 2-(1-imidazolyl)-4-(2-methoxyethyl)amino-6-(2-triethylsilylethynyl)quinazoline (prepn. given) with tetrabutylammonium fluoride afforded 6-ethynyl-4-(2-methoxyethyl)amino-2-(1-imidazolyl)quinazoline (II); II.2HCl demonstrated inhibition of cGMP-PDE with and TXA2 synthetase with IC50 = 4.6 + 10-8 and 2.4 + 10-6 M, resp. Pharmaceutical formulations were given.

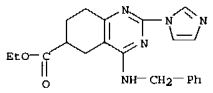
IT **157863-48-4P 157863-78-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(4-aminoquinazoline derivs. as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase)

RN 157863-48-4 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



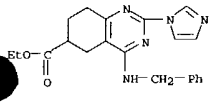
●2 HCl

RN 157863-78-0 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



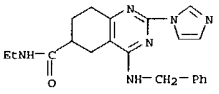
IT **157863-44-0P 157863-56-4P 157863-62-2P**
157863-79-1P 157863-80-4P 157863-88-2P
170986-00-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(4-aminoquinazoline derivs. as inhibitors of cyclic guanosine 3',5'-monophosphate phosphodiesterase and thromboxane A2 synthetase)

L3 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



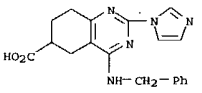
●2 HCl

RN 157863-80-4 CAPLUS
CN 6-Quinazolinecarboxamide, N-ethyl-5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



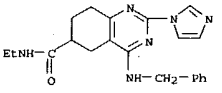
●2 HCl

RN 157863-88-2 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)

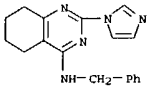


● Na

RN 170986-00-2 CAPLUS
CN 6-Quinazolinecarboxamide, N-ethyl-5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

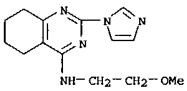


L3 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 157863-44-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(phenylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



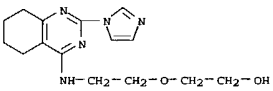
●2 HCl

RN 157863-56-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 157863-62-2 CAPLUS
CN Ethanol, 2-[2-[[5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-quinazolinyl]amino]ethoxy]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 157863-79-1 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

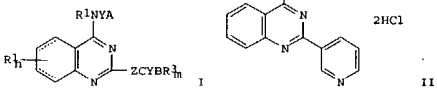
L3 ANSWER 27 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L3 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:605373 CAPLUS
DOCUMENT NUMBER: 121:205373
TITLE: 4-aminoquinazoline derivatives, and their use as medicine
INVENTOR(S): Lee, Sung Jai; Konishi, Yoshitaka; Macina, Orest Taras; Kondo, Kigen; Yu, Dingwei Tim
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 86 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 579496	A1	19940119	EP 1993-305557	19930715
EP 579496	B1	20011114		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 06192235	A2	19940712	JP 1993-197039	19930714
CA 2100626	AA	19940116	CA 1993-2100626	19930715
AT 208771	E	20011115	AT 1993-305557	19930715
ES 2167325	T3	20020516	ES 1993-305557	19930715
PT 579496	T	20020531	PT 1993-305557	19930715
JP 08099962	A2	19960416	JP 1995-264667	19950920
JP 2923742	B2	19990726		

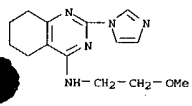
PRIORITY APPLN. INFO.: US 1992-913473 A 19920715
US 1993-76431 A 19930614
OTHER SOURCE(S): MARPAT 121:205373
GI



I II

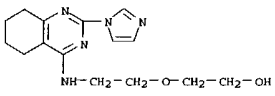
AB The title compds. I wherein R1 is H or alkyl; Y is bond or alkylene; A is (i) -CyAR2, (ii) -OR0 or -S(O)pR0, R0 = H, alkyl, etc., p is 0-2, (iii) -NR16R17, R16, R17 are H, alkyl; CyA is (1) a 3-7 membered monocyclic carbocyclic ring, (2) a 4-7 membered monocyclic hetero ring containing as hetero atoms, one N atom, one N and one O atoms, two N and one O atoms, or one N and two O atoms, (3) a 4-7 membered monocyclic hetero ring containing as hetero atoms, 1 or 2 O or S atoms, R2 is (1) H, (2) alkyl, (3) alkoxy, (4) -COOR5, in which R5 is H or alkyl, (5) -NR6R7, R6, R7 are H, alkyl, (6) -SO2NR6R7, (7) halogen, (8) CF3, (9) NO2 or (10) CF3O; Z is bond, methylene, ethylene, vinylene or ethynylene; CyB is a heterocyclic ring; R3 is H, alkyl, alkoxy, halogen or CF3; R4 is H, alkyl, alkoxy, etc., and acid addition salts thereof, salts thereof, and hydrates thereof were prepared

L3 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



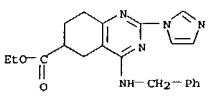
●2 HCl

RN 157863-62-2 CAPLUS
CN Ethanol, 2-[2-[[5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-quinazolinyl]amino]ethoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

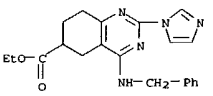


●2 HCl

RN 157863-78-0 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 157863-79-1 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

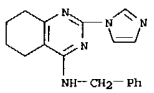


●2 HCl

L3 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
and have inhibitory effect on cGMP-PDE, or addnl. on TXA2 synthetase. Thus, a representative prepd. compd. II had inhibitory activity IC50 of 3.6 x 10-7 on cGMP-PDE.

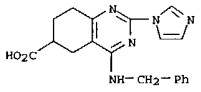
IT **157863-44-0P 157863-48-4P 157863-56-4P**
157863-62-2P 157863-78-0P 157863-79-1P
157863-80-4P 157863-88-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as cardiovascular agents)

RN 157863-44-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(phenylmethyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 157863-48-4 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)

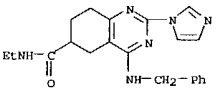


●2 HCl

RN 157863-56-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-N-(2-methoxyethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

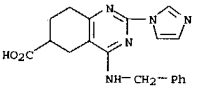
L3 ANSWER 28 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 157863-80-4 CAPLUS
CN 6-Quinazolinecarboxamide, N-ethyl-5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

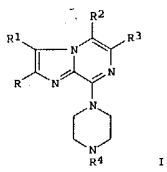
RN 157863-88-2 CAPLUS
CN 6-Quinazolinecarboxylic acid, 5,6,7,8-tetrahydro-2-(1H-imidazol-1-yl)-4-[(phenylmethyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)



● Na

L3 ANSWER 29 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:591811 CAPLUS
DOCUMENT NUMBER: 117:191811
TITLE: Synthesis and hypoglycemic activity of substituted 8-(1-piperazinyl)imidazo[1,2-a]pyrazines
AUTHOR(S): Meurer, Laura C.; Tolman, Richard L.; Chapin, Edward W.; Saperstein, Richard; Vicario, Pasquale P.; Zrada, Matthew M.; MacCoss, Malcolm
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(21), 3845-57
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

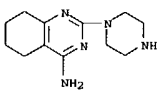


I

AB A series of alkyl- and halo-substituted 8-(1-piperazinyl)imidazo[1,2-a]pyrazines I (R, R2, R4 = H, Me; R1 = H, Cl, Me, Et, Pr, CHMe2, CH2CH2F; R3 = H, Cl, Me), were prepared using two approaches, the condensation of α-halocarbonyl derivs. RC(:X)CHR1Br with an aminopyrazine or the oxidation-dehydration of a [(β-hydroxyalkyl)amino]pyrazine. These imidazo[1,2-a]pyrazines were evaluated for their binding affinity to the α1, α2, β1, and β2 adrenergic receptors as well as their ability to lower blood glucose in insulin resistant hyperglycemic ob/ob mice. Modifications on 8-(1-piperazinyl)imidazo[1,2-a]pyrazine I (R-R4 = H)(II) reduced α2 binding, lowered hypoglycemic potency, and showed variations in binding to the α1, β1, and β2 adrenergic receptors. In addition to II, the 2-Me, 3-Me, and 5-Me 8-(1-piperazinyl)imidazo[1,2-a]pyrazines, resp.) displayed high affinity for the α2 receptor and were potent hypoglycemic agents when compared to 2-amino-7,8-dihydro-4-(1-piperazinyl)-6H-thiopyrano[3,2-d]pyramidine (MTP-1403). Receptor binding was modified by use of a 4-methylpiperazine moiety which reduced α1 and β1 binding while retaining some hypoglycemic activity. The structure-activity relationship for heterocyclic alkyl and halo substitution on biol. activity is discussed.

IT **79050-42-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(analogs of, preparation and hypoglycemic and adrenergic activity of)

RN 79050-42-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

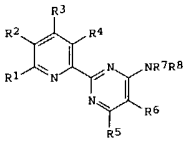


L3 ANSWER 30 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:429367 CAPLUS
DOCUMENT NUMBER: 115:29367
TITLE: Fungicidal pyridinylpyrimidinamines and their preparation
INVENTOR(S): Giencke, Wolfgang; Sachse, Burkhard; Wicke, Heinrich
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 89 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 407899	A2	19910116	EP 1990-112903	19900706
EP 407899	A3	19910724		
EP 407899	B1	19950301		
R: AT, CH, DE, ES, FR, GB, GR, IT, LI				
DE 3922735	A1	19910124	DE 1989-3922735	19890711
US 5250530	A	19931005	US 1990-549764	19900709
HU 54280	A2	19910228	HU 1990-4151	19900710

PRIORITY APPLN. INFO.: DE 1989-3922735 A 19890711
OTHER SOURCE(S): MARPAT 115:29367
GI

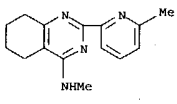


I

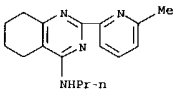
AB Title compds. I [R1 = H, alkyl, alkoxyalkyl, phenylalkyl, etc.; R2, R3, R4 = H, alkyl, (un)substituted phenyl; R5 = H, alkyl, cycloalkyl, alkoxy, alkylthio, etc.; R6 = H, alkyl, alkoxy, alkenyloxy, halo, (un)substituted Ph, etc.; R7, R8 = H, alkyl, alkoxyalkyl, phenylalkyl, etc.] were prepared as agricultural fungicides. Thus, 4-chloro-6-methyl-2-(2-methyl-6-pyridinyl)pyrimidine, PrNH2, K2CO3, and PhCH2N+Et3 Cl- were refluxed 7 h in MeCN to give 95% I (R1 = R5 = Me, R2 = R3 = R4 = R6 = R7 = H, R8 = Pr). When applied to barley plants at 500 mg/L of spray, several I showed 100% activity against organisms such as Erysiphe graminis.

IT **134543-94-5P 134543-97-8P 134544-00-6P**
134545-14-5P 134545-16-7P 134545-44-1P
134545-45-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as fungicide)

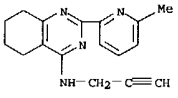
RN 134543-94-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-(6-methyl-2-pyridinyl)- (9CI) (CA INDEX NAME)



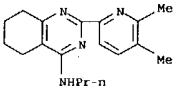
RN 134543-97-8 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(6-methyl-2-pyridinyl)-N-propyl- (9CI) (CA INDEX NAME)



RN 134544-00-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(6-methyl-2-pyridinyl)-N-2-propynyl- (9CI) (CA INDEX NAME)

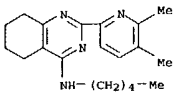


RN 134545-14-5 CAPLUS
CN 4-Quinazolinamine, 2-(5,6-dimethyl-2-pyridinyl)-5,6,7,8-tetrahydro-N-propyl- (9CI) (CA INDEX NAME)

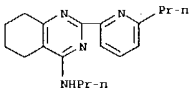


RN 134545-16-7 CAPLUS
CN 4-Quinazolinamine, 2-(5,6-dimethyl-2-pyridinyl)-5,6,7,8-tetrahydro-N-pentyl- (9CI) (CA INDEX NAME)

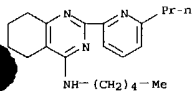
L3 ANSWER 30 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



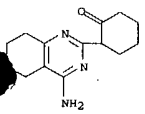
RN 134545-44-1 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-propyl-2-(6-propyl-2-pyridinyl)-(9CI) (CA INDEX NAME)



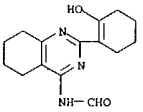
RN 134545-45-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-pentyl-2-(6-propyl-2-pyridinyl)-(9CI) (CA INDEX NAME)



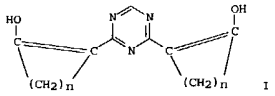
L3 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



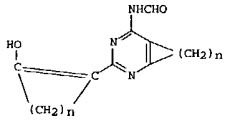
RN 121129-47-3 CAPLUS
CN Formamide, N-[5,6,7,8-tetrahydro-2-(2-hydroxy-1-cyclohexen-1-yl)-4-quinazolinyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 31 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:406684 CAPLUS
DOCUMENT NUMBER: 111:6684
TITLE: Synthesis and Dimroth rearrangement of 2,4-bis(2-hydroxy-1-cycloalkenyl)-1,3,5-triazines
AUTHOR(S): Honda, Itaru; Shimomura, Yoji
CORPORATE SOURCE: Fac. Eng., Fukui Univ., Fukui, Japan
SOURCE: Fukui Daigaku Kogakubu Kenkyu Hokoku (1988), 36(2), 165-81
CODEN: FDKHAD; ISSN: 0429-8373
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



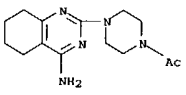
I



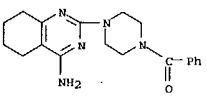
II

AB (Hydroxycycloalkenyl)triazines I (n = 4,5) were prepared by reaction of cyanuric chloride with enamine derivs. of the component cycloalkanone, followed by reductive hydrogenation of the resulting monochloro-1,3,5-triazines with PPh3 and I2. I were subjected to Dimroth rearrangement in EtOH-H2O and were converted into (hydroxycycloalkenyl)formylaminopyrimidine derivs. II. The mechanism of the Dimroth rearrangement was also proposed.
IT **121105-16-6P 121129-47-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 121105-16-6 CAPLUS
CN Cyclohexanone, 2-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:230 CAPLUS
DOCUMENT NUMBER: 100:230
TITLE: Pyrimidine derivatives. VII. Structure-activity relationship of hypoglycemic 4-amino-2-(1-piperazinyl)pyrimidines investigated by the adaptive least-squares method
AUTHOR(S): Sekiya, Tetsuo; Hata, Shunsuke; Yamada, Shun Ichi
CORPORATE SOURCE: Res. Lab., Mitsubishi Yuki Pharm. Co., Ltd., 300-03, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1983), 31(7), 2432-7
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Structure activity studies of 36 hypoglyemic 4-amino-2-(1-piperazinyl)-5,6-polymethylenepyrimidine derivs. I (R1 = NH2, NHBu, NEt2, pyrrolidino, etc.; R2 = H, Me, Ph, COPh, pyrrolidino, etc.; n = 3-5) were performed by the adaptive least-squares method. Apparently, the 2-(1-piperazinyl)pyrimidine moiety is an essential structure for the activity and the basicity of the 1-piperazinyl group is also important.
IT **76781-14-1 76781-15-2 76781-16-3**
76781-17-4 76781-18-5 76781-19-6
76781-20-9 76781-21-0 76781-22-1
76781-25-4 76781-26-5 76781-27-6
76781-28-7 76781-33-4 76781-34-5
76781-36-7 76781-43-6 76781-49-2
79050-42-3 88100-09-8 88100-10-1
88100-11-2 88100-12-3 88100-13-4
88100-14-5 88100-15-6
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hypoglycemic activity of, structure in relation to)
RN 76781-14-1 CAPLUS
CN Piperazine, 1-acetyl-4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)

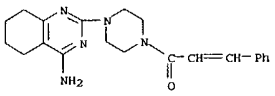


RN 76781-15-2 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-benzoyl- (9CI) (CA INDEX NAME)

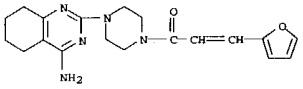


L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

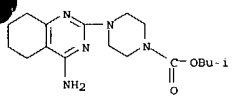
RN 76781-16-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



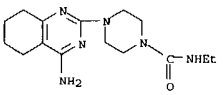
RN 76781-17-4 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(2-furanyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 76781-18-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

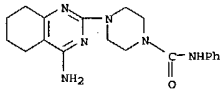


RN 76781-19-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-ethyl- (9CI) (CA INDEX NAME)

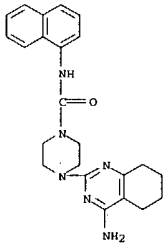


L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

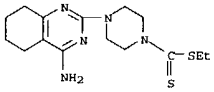
RN 76781-20-9 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-phenyl- (9CI) (CA INDEX NAME)



RN 76781-21-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-1-naphthalenyl- (9CI) (CA INDEX NAME)

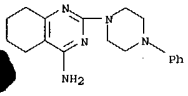


RN 76781-22-1 CAPLUS
CN 1-Piperazinecarbodithioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, ethyl ester (9CI) (CA INDEX NAME)

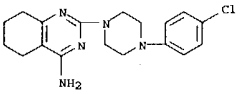


RN 76781-25-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

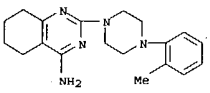
L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



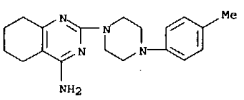
RN 76781-26-5 CAPLUS
CN 4-Quinazolinamine, 2-[4-(4-chlorophenyl)-1-piperazinyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 76781-27-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-methylphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

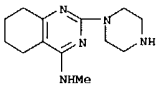


RN 76781-28-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(4-methylphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

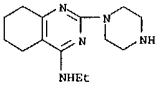


RN 76781-33-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

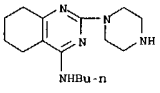
L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



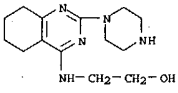
RN 76781-34-5 CAPLUS
CN 4-Quinazolinamine, N-ethyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)



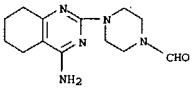
RN 76781-36-7 CAPLUS
CN 4-Quinazolinamine, N-butyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 76781-43-6 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(1-piperazinyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

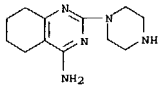


RN 76781-49-2 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)

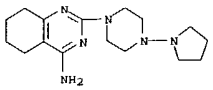


L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

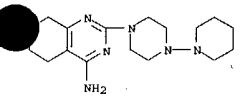
RN 79050-42-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)



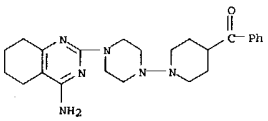
RN 88100-09-8 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(1-pyrrolidinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 88100-10-1 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(1-piperidinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



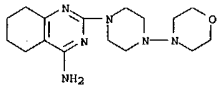
RN 88100-11-2 CAPLUS
CN Methanone, [1-[4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-1-piperazinyl]-4-piperidinyl]phenyl- (9CI) (CA INDEX NAME)



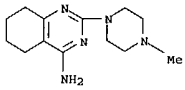
RN 88100-12-3 CAPLUS

L3 ANSWER 32 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

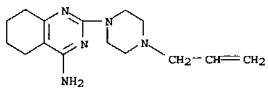
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(4-morpholinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



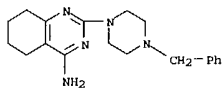
RN 88100-13-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



RN 88100-14-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-propenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 88100-15-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(phenylmethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

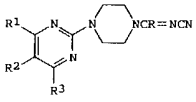


L3 ANSWER 33 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:104278 CAPLUS
DOCUMENT NUMBER: 96:104278
TITLE: Piperazinopyrimidines
PATENT ASSIGNEE(S): Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56135479	A2	19811022	JP 1980-38436	19800326
PRIORITY APPLN. INFO.:			JP 1980-38436	19800326

GI

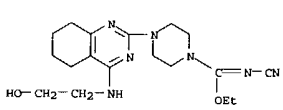


I

AB Piperazinopyrimidines I (R = alkoxy, alkylthio, alkylamino; R1, R2 = alkylene- or alkoxy-substituted benzene ring; R3 = dialkylamino, pyrrolidino, piperidino, morpholino) and their salts were prepared I are blockers for histaminic H2 receptors (0.1-1.5 g/day). Thus, treating 4-pyrrolidino-2-piperazino-5,6-tetramethylenepyrimidine with S,S-di-Me N-cyanoimidodithiocarbonate in EtOH 4-5 h at room temperature gave 4-pyrrolidino-2-[4-(methylthio-N-cyanoiminocarbonyl)piperazino]-5,6-tetramethylenepyrimidine.

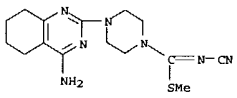
IT **81022-24-4P 81022-25-5P 81022-26-6P**
81022-28-8P 81022-30-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and histaminic acid H2 receptor blocking activity of)

RN 81022-24-4 CAPLUS
CN 1-Piperazinecarboximidic acid, N-cyano-4-[5,6,7,8-tetrahydro-4-[(2-hydroxyethyl)amino]-2-quinazolinyl]-, ethyl ester (9CI) (CA INDEX NAME)

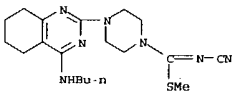


RN 81022-25-5 CAPLUS
CN 1-Piperazinecarboximidothioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-cyano-, methyl ester (9CI) (CA INDEX NAME)

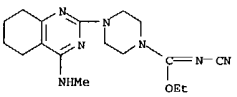
L3 ANSWER 33 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



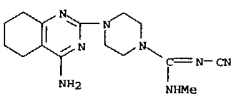
RN 81022-26-6 CAPLUS
CN 1-Piperazinecarboximidothioic acid, 4-[4-(butylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]-N-cyano-, methyl ester (9CI) (CA INDEX NAME)



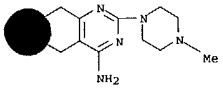
RN 81022-28-8 CAPLUS
CN 1-Piperazinecarboximidic acid, N-cyano-4-[5,6,7,8-tetrahydro-4-(methylamino)-2-quinazolinyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 81022-30-2 CAPLUS
CN 1-Piperazinecarboximidamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-cyano-N'-methyl- (9CI) (CA INDEX NAME)



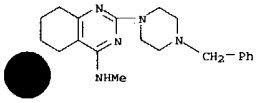
L3 ANSWER 34 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:532796 CAPLUS
DOCUMENT NUMBER: 95:132796
TITLE: Pyrimidine derivatives. II. New synthesis and reactions of 4-amino-2-methylthiopyrimidine derivatives
AUTHOR(S): Sekiya, Tetsuo; Hiranuma, Hidetoshi; Uchide, Masayuki; Hata, Shunsuke; Yamada, Shunichi
CORPORATE SOURCE: Res. Lab., Mitsubishi Pharm. Co., Ltd., Ibaraki, 300-03, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1981), 29(4), 948-54.
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:132796
GI For diagram(s), see printed CA Issue.
AB Oxidation of pyrimidines I [RR1 = (CH2)n, n = 3-5; R2 = SOmMe, m = 0], prepared by cyclocondensation of RCOCH2R1 with H2NC(SMe):NCN, gave I (m = 1, 2). Aminating I [RR1 = (CH2)4, R2 = SOMe] with NH3, MeNH2, and pyrrolidine gave II (R2 = NH2, NHMe, pyrrolidino). Quinazolinones III (n = 3, 4) were prepared by treating I [RR1 = (CH2)n, n = 3, 4; R2 = SMe] with NaNO2 or isoamyl nitrite.
IT **79050-43-4P 79050-46-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzylation of)
RN 79050-43-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methyl-1-piperazinyl)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

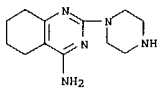
RN 79050-46-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(phenylmethyl)-1-piperazinyl]-, hydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 34 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



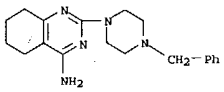
●2 HCl

RN 79051-13-1 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)-, hydrochloride (9CI) (CA INDEX NAME)



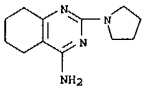
●x HCl

L3 ANSWER 34 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

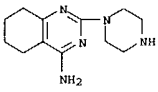


●x HCl

IT **76781-07-2P 79050-42-3P 79051-12-0P 79051-13-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 76781-07-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 79050-42-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

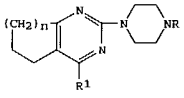


RN 79051-12-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:425129 CAPLUS
DOCUMENT NUMBER: 95:25129
TITLE: Pharmaceutical 5,6-alkylenepyrimidine derivatives
INVENTOR(S): Hiranuma, Hidetoshi; Mizogami, Susumu; Mori, Motokuni; Sekiya, Tetsuo; Kanayama, Toshiji; Hanatsuka, Mitsuo
PATENT ASSIGNEE(S): Mitsubishi Yuka Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 22481	A1	19810121	EP 1980-103456	19800620
R: BE, DE, FR, GB, IT				
JP 56002968	A2	19810113	JP 1979-77582	19790621
JP 56090070	A2	19810721	JP 1979-166792	19791224
JP 63038997	B4	19880803		
US 4352928	A	19821005	US 1980-160080	19800616
PRIORITY APPLN. INFO.:			JP 1979-77582 A	19790621
			JP 1979-166792 A	19791224

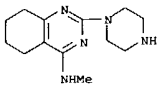
OTHER SOURCE(S): CASREACT 95:25129
GI



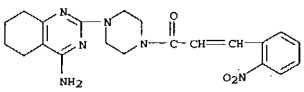
I

AB Piperazinopyrimidines I (n = 1-3; R = H, alkyl, optionally substituted CH2Ph, acyl, thioacyl, carbamoyl, PhSO2, heterocyclic; R1 = amino, alkoxy, aryloxy) were prepared Thus, 2-chloro-4-amino-5,6-tetramethylenepyrimidine was treated with N-formylpiperazine and deformylated to give I (R = H, R1 = NH2, n = 2). At 30 mg/kg orally in mice I (R = H, R1 = NH2, n = 2) caused 67.8% decrease in blood sugar level and at 100 μM caused 100% inhibition of blood platelet aggregation. Other I had antiinflammatory and antidiabetic activity.
IT **76781-33-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antidiabetic and platelet aggregation-inhibiting activity of)
RN 76781-33-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

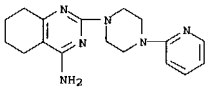
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **78042-02-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antihypertensive activity of)
RN 78042-02-1 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(2-nitrophenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

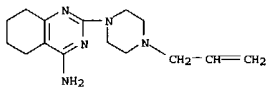


IT **78042-13-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antihypertensive and antidiabetic activity of)
RN 78042-13-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-pyridinyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



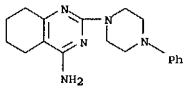
IT **76781-13-0P 76781-25-4P 78042-11-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiinflammatory activity of)
RN 76781-13-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-propenyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

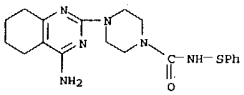


●2 HCl

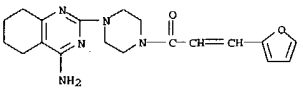
RN 76781-25-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



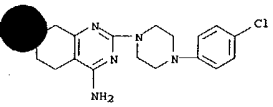
RN 78042-11-2 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-(phenylthio)- (9CI) (CA INDEX NAME)



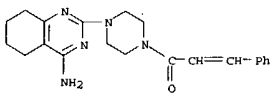
IT **76781-17-4P 76781-26-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiinflammatory and antidiabetic activity of)
RN 76781-17-4 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(2-furanyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



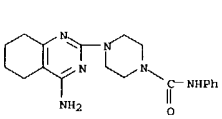
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 76781-26-5 CAPLUS
CN 4-Quinazolinamine, 2-[4-(4-chlorophenyl)-1-piperazinyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



IT **76781-16-3P 78042-07-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiinflammatory and antihypertensive activity of)
RN 76781-16-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)



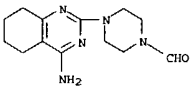
RN 78042-07-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-phenyl-, hydrochloride (9CI) (CA INDEX NAME)



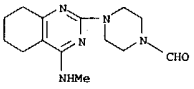
●x HCl

IT **76781-49-2P 76781-50-5P 76781-51-6P 76781-52-7P 76781-57-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deformylation of)
RN 76781-49-2 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)

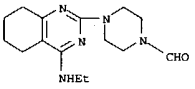
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



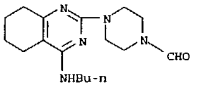
RN 76781-50-5 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[5,6,7,8-tetrahydro-4-(methylamino)-2-quinazolinyl]- (9CI) (CA INDEX NAME)



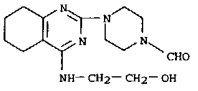
RN 76781-51-6 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-(ethylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 76781-52-7 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-(butylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 76781-57-2 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[5,6,7,8-tetrahydro-4-[(2-hydroxyethyl)amino]-2-quinazolinyl]- (9CI) (CA INDEX NAME)

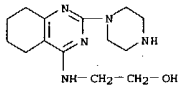


L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **78042-20-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platelet aggregation inhibiting activity of)
RN 78042-20-3 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(1-piperazinyl)-4-quinazolinyl]amino]-, compd. with 2,4,6-trinitrophenol (9CI) (CA INDEX NAME)

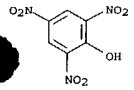
CM 1

CRN 76781-43-6
CMF C14 H23 N5 O



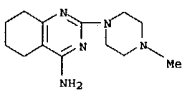
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



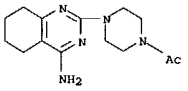
IT **76781-11-8P 76781-14-1P 76781-15-2P**
76781-18-5P 76781-19-6P 76781-21-0P
76781-22-1P 76781-23-2P 76781-24-3P
76781-28-7P 76781-34-5P 78042-01-0P
78042-03-2P 78042-04-3P 78042-05-4P
78042-06-5P 78042-08-7P 78042-09-8P
78042-10-1P 78042-12-3P 78042-14-5P
78042-18-9P 78043-18-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 76781-11-8 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

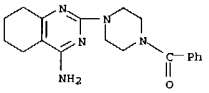


●2 HCl

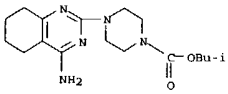
RN 76781-14-1 CAPLUS
CN Piperazine, 1-acetyl-4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)



RN 76781-15-2 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-benzoyl- (9CI) (CA INDEX NAME)

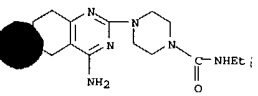


RN 76781-18-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

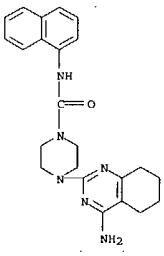


RN 76781-19-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-

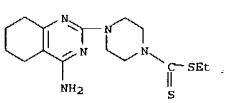
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
ethyl- (9CI) (CA INDEX NAME)



RN 76781-21-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-1-naphthalenyl- (9CI) (CA INDEX NAME)

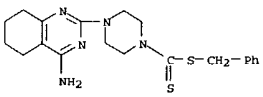


RN 76781-22-1 CAPLUS
CN 1-Piperazinecarbodithioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, ethyl ester (9CI) (CA INDEX NAME)

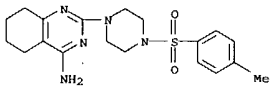


RN 76781-23-2 CAPLUS
CN 1-Piperazinecarbodithioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

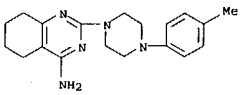
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



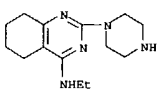
RN 76781-24-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 76781-28-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(4-methylphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

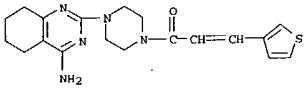


RN 76781-34-5 CAPLUS
CN 4-Quinazolinamine, N-ethyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

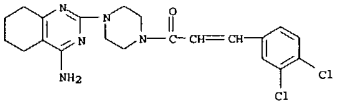


RN 78042-01-0 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[1-oxo-3-(3-thienyl)-2-propenyl]- (9CI) (CA INDEX NAME)

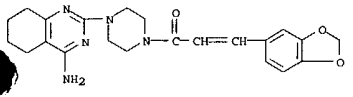
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



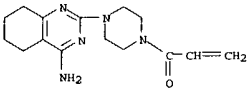
RN 78042-03-2 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(3,4-dichlorophenyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 78042-04-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(1,3-benzodioxol-5-yl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

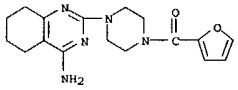


RN 78042-05-4 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(1-oxo-2-propenyl)- (9CI) (CA INDEX NAME)

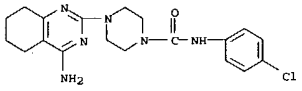


RN 78042-06-5 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(2-furanylcarbonyl)- (9CI) (CA INDEX NAME)

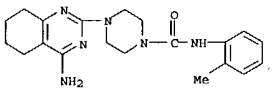
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 78042-08-7 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-(4-chlorophenyl)- (9CI) (CA INDEX NAME)

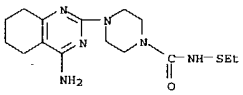


RN 78042-09-8 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-(2-methylphenyl)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

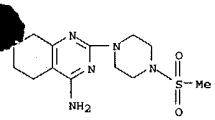
RN 78042-10-1 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-(ethylthio)-, hydrochloride (9CI) (CA INDEX NAME)



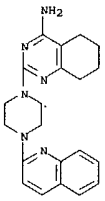
●x HCl

L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 78042-12-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(methylsulfonyl)- (9CI) (CA INDEX NAME)



RN 78042-14-5 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-quinolinyl)-1-piperazinyl]-, hydrochloride (9CI) (CA INDEX NAME)

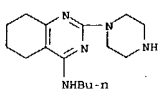


●x HCl

RN 78042-18-9 CAPLUS
CN 4-Quinazolinamine, N-butyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)-, compd. with 2,4,6-trinitrophenol (9CI) (CA INDEX NAME)

CM 1

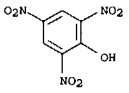
CRN 76781-36-7
CMF C16 H27 N5



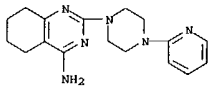
CM 2

L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CRN 88-89-1
CMF C6 H3 N3 O7

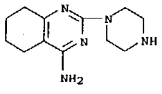


RN 78043-18-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-pyridinyl)-1-piperazinyl]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

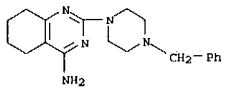
IT **76781-32-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, acylation, and pharmacol. activity of)
RN 76781-32-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

IT **76781-12-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, debenzylation, and antiinflammatory activity of)
RN 76781-12-9 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)

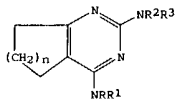
L3 ANSWER 35 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 HCl

L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:139724 CAPLUS
DOCUMENT NUMBER: 94:139724
TITLE: Pyrimidine derivatives I. Synthesis of hypoglycemic 2-piperazino-5,6-polymethylenepyrimidines
AUTHOR(S): Sekiya, Tetsuo; Hiranuma, Hidetoshi; Kanayama, Toshiji; Hata, Shunsuke
CORPORATE SOURCE: Res. Lab., Mitsubishi Yuka Pharm. Co., Ltd., Ibaraki, 300-03, Japan
SOURCE: European Journal of Medicinal Chemistry (1980), 15(4), 317-22
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 94:139724
GI

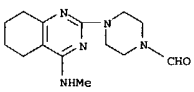


I

AB Cycloalkanopyrimidinediamines I (n = 1-3; R = H, R1 = H, Me, Et, Bu, CH2CH2OH; NRR1 = NMe2, NEt2, morpholino, pyrrolidino; NR2R3 = pyrrolidino, piperidino, 4-benzylpiperidino, morpholino, optionally substituted piperazino) (36 compds.) were prepared by aminating dichlorocycloalkanopyrimidines, prepared by treating 2-ethoxycarbonylcycloalkanones with urea and chlorinating the resulting uracils. I had hypoglycemic activity which is most potent in I (NR2R3 = optionally substituted piperazino). Some I also have blood platelet aggregation-inhibiting activity.

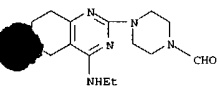
IT **76781-50-5P 76781-51-6P 76781-52-7P**
76781-57-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deformylation of)

RN 76781-50-5 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[5,6,7,8-tetrahydro-4-(methylamino)-2-quinazolinyl]- (9CI) (CA INDEX NAME)

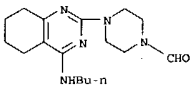


RN 76781-51-6 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-(ethylamino)-5,6,7,8-tetrahydro-2-

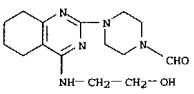
L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
quinazolinyl]- (9CI) (CA INDEX NAME)



RN 76781-52-7 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[4-(butylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]- (9CI) (CA INDEX NAME)



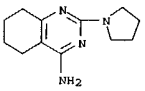
RN 76781-57-2 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-[5,6,7,8-tetrahydro-4-[(2-hydroxyethyl)amino]-2-quinazolinyl]- (9CI) (CA INDEX NAME)



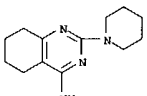
IT **76781-07-2P 76781-08-3P 76781-09-4P**
76781-10-7P 76781-11-8P 76781-12-9P
76781-13-0P 76781-14-1P 76781-15-2P
76781-16-3P 76781-17-4P 76781-18-5P
76781-19-6P 76781-20-9P 76781-21-0P
76781-22-1P 76781-23-2P 76781-24-3P
76781-25-4P 76781-26-5P 76781-27-6P
76781-28-7P 76781-35-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and hypoglycemic activity of)

RN 76781-07-2 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

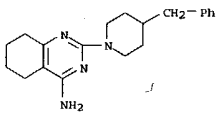
L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 76781-08-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperidinyl)- (9CI) (CA INDEX NAME)

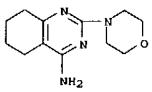


RN 76781-09-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(phenylmethyl)-1-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)



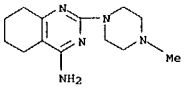
● HCl

RN 76781-10-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-morpholinyl)- (9CI) (CA INDEX NAME)



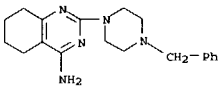
RN 76781-11-8 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



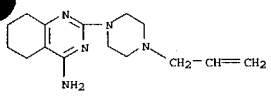
●2 HCl

RN 76781-12-9 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(phenylmethyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

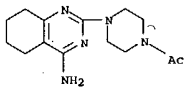
RN 76781-13-0 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-propenyl)-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



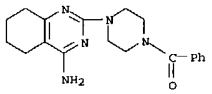
●2 HCl

RN 76781-14-1 CAPLUS
CN Piperazine, 1-acetyl-4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)

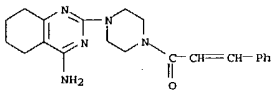
L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



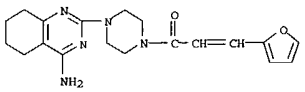
RN 76781-15-2 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-benzoyl- (9CI) (CA INDEX NAME)



RN 76781-16-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-(1-oxo-3-phenyl-2-propenyl)- (9CI) (CA INDEX NAME)

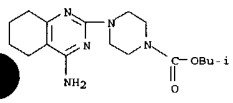


RN 76781-17-4 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[3-(2-furanyl)-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

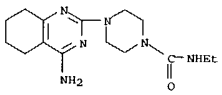


RN 76781-18-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, 2-methylpropyl ester (9CI) (CA INDEX NAME)

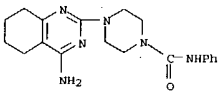
L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 76781-19-6 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-ethyl- (9CI) (CA INDEX NAME)

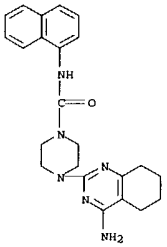


RN 76781-20-9 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-phenyl- (9CI) (CA INDEX NAME)

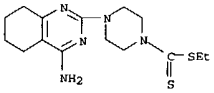


RN 76781-21-0 CAPLUS
CN 1-Piperazinecarboxamide, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-N-1-naphthalenyl- (9CI) (CA INDEX NAME)

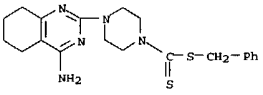
L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



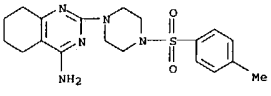
RN 76781-22-1 CAPLUS
CN 1-Piperazinecarbodithioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 76781-23-2 CAPLUS
CN 1-Piperazinecarbodithioic acid, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

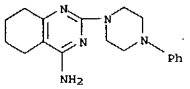


RN 76781-24-3 CAPLUS
CN Piperazine, 1-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)-4-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

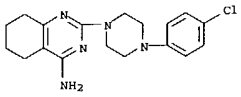


L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

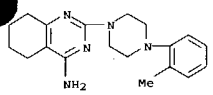
RN 76781-25-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(4-phenyl-1-piperazinyl)- (9CI) (CA INDEX NAME)



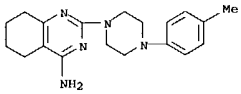
RN 76781-26-5 CAPLUS
CN 4-Quinazolinamine, 2-[4-(4-chlorophenyl)-1-piperazinyl]-5,6,7,8-tetrahydro- (9CI) (CA INDEX NAME)



RN 76781-27-6 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(2-methylphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)

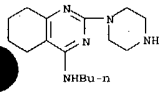


RN 76781-28-7 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-[4-(4-methylphenyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



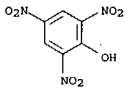
RN 76781-35-6 CAPLUS

L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



CM 2

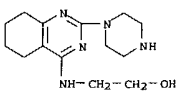
CRN 88-89-1
CMF C6 H3 N3 O7



RN 76781-44-7 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(1-piperazinyl)-4-quinazolinyl]amino]-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

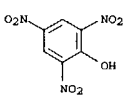
CM 1

CRN 76781-43-6
CMF C14 H23 N5 O



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

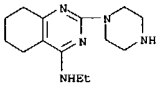


IT **76781-32-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Quinazolinamine, N-ethyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)-, ethanedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

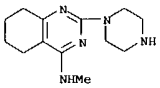
CRN 76781-34-5
CMF C14 H23 N5



CM 2

CRN 144-62-7
CMF C2 H2 O4

IT **76781-33-4P 76781-37-8P 76781-44-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and pharmacol. activity of)
RN 76781-33-4 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-(1-piperazinyl)- (9CI) (CA INDEX NAME)

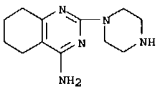


RN 76781-37-8 CAPLUS
CN 4-Quinazolinamine, N-butyl-5,6,7,8-tetrahydro-2-(1-piperazinyl)-, compd. with 2,4,6-trinitrophenol (1:2) (9CI) (CA INDEX NAME)

CM 1

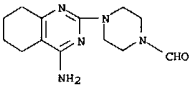
CRN 76781-36-7
CMF C16 H27 N5

L3 ANSWER 36 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(prepn., acylation, and pharmacol. activity of)
RN 76781-32-3 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

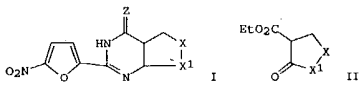


●2 HCl

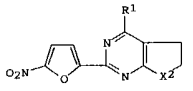
IT **76781-49-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, deformylation, and hypoglycemic activity of)
RN 76781-49-2 CAPLUS
CN 1-Piperazinecarboxaldehyde, 4-(4-amino-5,6,7,8-tetrahydro-2-quinazolinyl)- (9CI) (CA INDEX NAME)



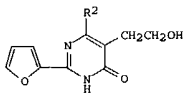
L3 ANSWER 37 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:29739 CAPLUS
DOCUMENT NUMBER: 86:29739
TITLE: Chemotherapeutic nitroheterocycles. 25. 2-(5-Nitro-2-furyl)-5,6,7,8-tetrahydroquinazolines and related compounds
AUTHOR(S): Albrecht, R.; Schumann, K.
CORPORATE SOURCE: Forschungslab., Schering A.-G., Berlin, Fed. Rep. Ger.
SOURCE: European Journal of Medicinal Chemistry (1976), 11(2), 155-8
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 86:29739
GI


I

II

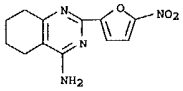

III


IV

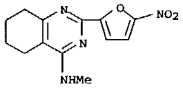

V

AB Fused pyrimidines I [XX1 = (CH2)2, (CH2)3, NBuCH2CH2; Z = O] were prepared by treating 2-furamidine-HCl with NaOEt and II and nitrating the product. Chlorination of I [XX1 = (CH2)3] gave quinazoline III, which was aminated to give III [R = NH2, NHMe, pyrrolidino-HCl, morpholino-HCl, NHCH2CH2NMe2-2HCl; X2 = (CH2)2]. 2-Furamidine-HCl and furanones IV (R2 = CO2Et, Ac, cyano) gave pyrimidinones V (R2 = OH, Me, NH2), which were cyclized with concentrated H2SO4 and the products nitrated to give III (R1 = R2 of V, X2 = O). Also prepared was I [XX1 = (CH2)2, Z = S]. III (R1 = Cl, Me, basic substituent) had min. inhibitory concns. against Trichomonas vaginolis of 0.05-1.6 μg/ml.
IT **61378-95-8P 61378-96-9P 61378-98-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and trichomonocidal activity of)
RN 61378-95-8 CAPLUS

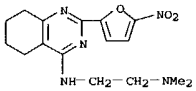
L3 ANSWER 37 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)



RN 61378-96-9 CAPLUS
CN 4-Quinazolinamine, 5,6,7,8-tetrahydro-N-methyl-2-(5-nitro-2-furanyl)- (9CI) (CA INDEX NAME)

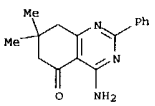


RN 61378-98-1 CAPLUS
CN 1,2-Ethanediamine, N,N-dimethyl-N'-[5,6,7,8-tetrahydro-2-(5-nitro-2-furanyl)-4-quinazolinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

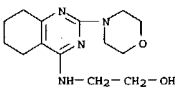
L3 ANSWER 38 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:492147 CAPLUS
DOCUMENT NUMBER: 79:92147
TITLE: Synthesis of some heterocycles from 2-cyano-3-ethoxy-5,5-dimethyl-2-cyclohexen-1-one
AUTHOR(S): Strakov, A. Ya.; Andaburskaya, M. B.; Moiseenkov, A. M.; Akhrem, A. A.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1973), (3), 330-2
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB The title compound (I) cyclized with PhC(:NH)NH2, N2H4, and PhNHNH2 to give tetrahydroquinazolinone II and tetrahydroindazoles III and IV, resp.; I and HONH2 yielded the tautomeric benzisoxazoles V and VI.
IT **43103-05-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 43103-05-5 CAPLUS
CN 5(6H)-Quinazolinone, 4-amino-7,8-dihydro-7,7-dimethyl-2-phenyl- (9CI) (CA INDEX NAME)



L3 ANSWER 39 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:119485 CAPLUS
DOCUMENT NUMBER: 78:119485
TITLE: Pharmacologically active pyrimidine derivatives
PATENT ASSIGNEE(S): UCB (Union Chimique-Chemische Bedrijven), S. A.
SOURCE: Fr. M., 6 pp. Division of Fr. 1,555,899 (See Brit. 1,152,853 CA 71:112965r).
CODEN: FMXXAJ
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

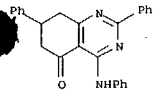
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 7575		19700216		
PRIORITY APPLN. INFO.:			GB 1967-3775	19670125

AB The cardiovascular, bronchodilating, and spasmolytic activity of twenty-six 4,5-polymethylenepyrimidine derivs. was studied. 2-Propyl-4,5-tetramethylene-6-morpholinopyrimidine (I) [23920-44-7], with coronary and peripheral vasodilating, bronchodilating, and spasmolytic activities greater than those of theophylline [58-55-9], appeared to be the most active compound
IT **23902-11-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of)
RN 23902-11-6 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(4-morpholinyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

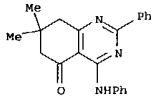


10/ 674,350

L3 ANSWER 40 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1970:435316 CAPLUS
DOCUMENT NUMBER: 73:35316
TITLE: 2-Phenyl-7,7-dimethyl- and 2,7-diphenyl-4-phenylamino-5-oxo-5,6,7,8-tetrahydroquinazoline
AUTHOR(S): Strakov, A. Ya.; Brutane, D.; Deich, V. D.
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1970), (2), 248-9
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB 5,5-Dimethyl- (Ia) and 5-phenyl-2-(phenylthiocarbamoyl)-1,3-hexanedione (Ib) yield, by the action of benzamidine (II), the corresponding 3-(N-benzamidinyl)-2-(phenylthiocarbamoyl)-2-cyclohexen-1-ones (IIIa, IIIb), which undergo cyclization to 2-phenyl-7,7-dimethyl- (IVa) or 2,7-diphenyl-4-(phenylamino)-5-oxo-5,6,7,8-tetrahydroquinazoline (IVb). Ib (40%), m. 151-3°, was prepared from 5-phenyl-1,3-cyclohexanedione and PhNCS. The reaction of Ia and Ib with II.HCl in EtOH-EtONa yielded, after boiling, IIIa (10 min, 55%, m. 174°) and IIIb [2 hr, 59%, m. 180-4° (decomposition)]. The ring closure was performed in boiling dioxane with several drops H3PO4 to give 57% IVa, m. 137-9°, and 50% IVb, m. 203-7° (decomposition).
IT **27351-00-4P 27351-01-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27351-00-4 CAPLUS
CN 5(6H)-Quinazolinone, 4-anilino-7,8-dihydro-2,7-diphenyl- (8CI) (CA INDEX NAME)



RN 27351-01-5 CAPLUS
CN 5(6H)-Quinazolinone, 4-anilino-7,8-dihydro-7,7-dimethyl-2-phenyl- (8CI) (CA INDEX NAME)



L3 ANSWER 41 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:512965 CAPLUS
DOCUMENT NUMBER: 71:112965
TITLE: Therapeutic 4,5-alkylenepyrimidine derivatives
INVENTOR(S): Mathieu, Jacques
PATENT ASSIGNEE(S): UCB(Union Chimique-Chemische Bedrijven), S. A.
SOURCE: Brit., 9 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1152883		19690521	GB	19670125
DE 1695974			DE	
FR 1555899			FR	
FR 7575			FR	
US 3757017		19730000	US	

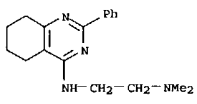
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), hypotensives, peripheral and coronary vasodilators, diuretics, bronchodilators, spasmolytics, and circulatory and respiratory analeptics, are prepared Thus, a mixture of 42.1 g. I (R = Pr, R1 = Cl, n = 4) (IIa) and 70 g. morpholine (III) is heated 5 hrs. at 130° to give 92.5% I (R = Pr, R1 = morpholino, n = 4) (Ia), b0.005 142-4°, m. 60°; Ia.HCl m. 191° (Et2O). Na (16.2 g.)was dissolved in 400 ml. MeOH, 39 g. PrC(:NH)NH2.HC l and 56.5 g. 2-carbethoxycycloheptanone added, and the mixture refluxed 14 hrs. to give 92% I (R = Pr, R1 = OH, n = 5) (IIb), m. 170°. Similarly obtained are IIb analogs: n = 3, m. 213-14°; n = 4, m. 127°. IIb (103 g.) in 500 ml. POCl3 is refluxed 5 hrs., and worked up to give 92% I (R = Pr, R1 = Cl, n = 5) (IIc), b0.005 111-12°. Similarly prepared are: IIa, b0.001 92-3°, m. 39.5-40.5°; I (R = Pr, R1 = Cl, n = 3), b0.002 90-1°. A mixture of 22.4 g. IIc and 177.4 g. III in 100 ml. anhydrous dioxane is refluxed 16 hrs. to give 88% I (R = Pr, R1 = morpholino, n = 5) (Ib), b0.001 144-6°; Ib.HCl m. 210-11° (Et2O). I (R1 = morpholino) similarly obtained are (R and n given): Me, 4(Ic) (b0.001 129-33°, m. 71-2°); iso-Bu, 4(Id) [HCl salt m. 157-8° (Et2O)]; pentyl, 4 [HCl salt m. 127-8° (Et2O)]; Pr, 3 (Ie) (b0.001 152 3°, R1 = I m. 53-4°); Pr, 6 (If) [HCl salt m. 163-4° (Et2O)]. Also prepared were HOC2H4NH (R and n given): Me, 4 (m. 148-9°); iso-Bu 4 [m. 159-60° (EtOAc-hexane)]; pentyl, 4 [m. 125-6° (EtOAc-hexane)]; Pr, 3 [m. 126-7° (EtOAc-hexane)]; Pr, 4 (m. 134° (EtOAc-hexane)]; Pr, 5 (Ig) (m. 142-3°); Pr, 6 (Ih), [m. 153-4° (EtOAc-hexane)]. Also prepared was I (R = HOC2H4NMe, R1 = Pr, n = 4 (Ii) b0.2 128-30°, n21D 1.5184, unstable), and I [R1 = (HOC2H4)2N]; (R and n given): Pr, 3 (Ij) [m. 111-12° (EtOAc-hexane)]; Pr, 5 [m. 67-8° (hexane)]. A solution of 20.3 g. I (R = R1 = Cl, n = 4) (IId) in 50 ml. anhydrous dioxane is mixed with 17.4 g. III in 50 ml. anhydrous dioxane and the mixture stirred 2 hrs. to give 79% I (R = Cl, R1 = morpholino, n = 4) (Ik), m. 180°; for comparison, I (R = morpholino, R1 = Cl, n = 4) (Il), m. 113-14° is prepared by refluxing POCl3 with I (R = morpholino, R1 = OH, n = 4) (Im), m. 214-15°, itself prepared from morpholinoformamidine, 2-carboxycyclohexanone, and NaOMe in MeOH. Il and Im were not therapeutic

L3 ANSWER 41 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
compds. Il may be dechlorinated to give I (R = morpholino, R1 = H, n = 4) (In) [HCl salt m. 185-6° (iso-Pr2O)] by the method used for It. Similarly prepd. to Ik are I (R = Cl, R1 = HOC2H4NH, n = 4) (Io), m. 138-9° (EtOAc-hexane), and I [R = Cl, R2 = (HOC2H4)2N, n = 4] m. 80° (aq. EtOH). A mixt. of 12.4 g. IId and 106 g. III, is heated 14 hrs. at 130°, to give 77% I (R = R1 = morpholino, n = 4) m. 112-13° (EtOAc-hexane). Io (6.5 g.) and 25 g. III is heated 16 hrs. at 130° to give 85% I (R = morpholino, R1 = HOC2H4, n = 4) m. 126-7°. A soln. of 8 g. II (R = H, R1 = Cl, n = 4) (IIe) and 5.8 g. HOC2H4NH2 in 100 ml. anhyd. dioxane is refluxed 30 hrs. and cooled, and the org. layer filtered through Hyflocel and evapd. to give 73.5% I (R = H, R1 = HOC2H4, n = 4) m. 131-2°. A mixt. of 7.6 g. Ik and 3 g. 5% Pd-C in 200 ml. EtOH is hydrogenated 2 hrs. at room temp./1 atm., and worked up to give 6.3 g. I (R = H, R1 = morpholino, n = 4); It.HCl m. 223-4° (1:1 iso-PrOH-iso-Pr2O) and is also prepd. from IIe and III. A mixt. of 20.3 g. IId and 61 g. HOC2H4NH2 is heated 7 hrs. at 150-60° to give 60% I (R = R1 = HOC2H4, n = 4), m. 133-4° (Me2CO-Et2O). The results of biol. tests are given.
IT **23902-11-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23902-11-6 CAPLUS
CN Ethanol, 2-[[5,6,7,8-tetrahydro-2-(4-morpholinyl)-4-quinazolinyl]amino]- (9CI) (CA INDEX NAME)

L3 ANSWER 42 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:105236 CAPLUS
DOCUMENT NUMBER: 68:105236
TITLE: Tetrahydroquinazolines
INVENTOR(S): Carney, Richard W. J.; Blatter, Herbert M.; De Stevens, George
PATENT ASSIGNEE(S): CIBA Corp.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

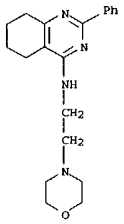
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3346452		19671010	US	19630819

GI For diagram(s), see printed CA Issue.
AB Analgesic agents are described which consist of the general formula I, where R = H or a lower alkyl, aryl, aralkyl, or heterocyclic radical; R1 = H lower alkyl, aralkyl, or acyl; n = preferably 2-3; Q = an N,N-disubstituted amino group. Salts, N-oxides, N-oxide salts, and quaternary ammonium bases of I can also be analgesic. Intermediates for the preparation have preferably the general formula (II). Thus, to 107 g. BzN:C:S, prepared as described by Dixon et al. (1908), in 150 ml. CHCl3 and 55.0 g. 1-morpholinocyclohexene in 45 ml. CHCl3, was added at 5° over 1 hr. under N, and the mixture refluxed 30 min. and kept over night to precipitate red 2-phenyl-5,6,7,8-tetrahydro-4H-1,3-benzoxazine-4-thione (III), needles, m. 197-9° (HCONMe2). NH3 was bubbled through a solution of 4.0 g. III in 100 ml. MeOH. After 1 hr. the solvent was removed to yield 86% 2-phenyl-1,4,5,6,7,8-hexahydroquinazoline-4-thione (IV), m. 199-20° (EtOH). A mixture of 1.0 g. IV and 10 ml. POCl3 was refluxed 1 hr., cooled, poured into ice, and extracted with CHCl3 to give 67% 4-chloro-2-phenyl-5,6,7,8-tetrahydroquinazoline (V), m. 105-6° (EtOH). A mixture of 2.0 g. V and 3.2 g. Me2N(CH2)2NH2 was refluxed 2 hrs., cooled, poured into H2O, and allowed to stand to yield 79% I (R = Ph, R1 = H, Q = Me2N, n = 2), m. 87-90° (MeCN). Other compds. prepared were I (R = Ph, R1 = H, Q = morpholino, n = 2), m. 109-10° (MeCN), I (R = R1 = H, Q = Me2N, n = 2, m. 98-101° (pentane), and as intermediates 4-chloro-5,6,7,8-tetrahydroquinazoline (84-7°) and its hydrobromide, m. 210-13° (MeOH-Et2O).
IT **17709-74-9P 17709-78-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 17709-74-9 CAPLUS
CN Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-5,6,7,8-tetrahydro-2-phenyl- (7CI, 8CI) (CA INDEX NAME)



RN 17709-78-3 CAPLUS
CN Quinazoline, 5,6,7,8-tetrahydro-4-[(2-morpholinoethyl)amino]-2-phenyl- (7CI, 8CI) (CA INDEX NAME)

L3 ANSWER 42 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L3 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1968:87308 CAPLUS
DOCUMENT NUMBER: 68:87308
TITLE: Bicyclic diaza compounds
INVENTOR(S): Carney, Richard W. J.; Blatter, Herbert M.; De Stevens, George
PATENT ASSIGNEE(S): CIBA Corp.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3322759		19670530	US	19660302

GI For diagram(s), see printed CA Issue.

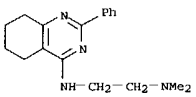
AB A mixture of 2.0 g. chloro-2-phenyl-5,6,7,8-tetrahydroquinazoline and 3.2 g. N,N-dimethylethylenediamine was refluxed 2 hrs. After cooling, it was poured into H2O and allowed to stand to give 4-N-(2-N,N-dimethylaminoethyl)-2-phenyl-5,6,7,8-tetrahydroquinazoline (I), m. 82-90° (MeCN). A solution of 0.5 g. I in a small amount EtOH was treated with a saturated HCl solution in EtOH and then diluted with Et2O to yield I.2 HCl. The picrate was also prepared A solution of 107 g. N-benzoyl isothiocyanate in 150 cc. CHCl3 was cooled to 5° and then treated with 55 g. of 1-morpholinocyclohexene in 45 cc. CHCl3. The solution was added over 1 hr. with cooling in N atmospheric After removing the ice bath, the mixture was refluxed 30 min. and then allowed to stand overnight and 2-phenyl-5,6,7,8-tetrahydro-4H-1,3-benzoxazine-4-thione (II) was filtered off and washed with Et2O and MeOH to yield 3.8 g. red needles, m. 197-9° (HCONMe2). NH3 gas was bubbled through a solution of 4.0 g. II in 100 cc. MeOH. After 1 hr., the solvent was removed to give 2-phenyl-1,4,5,6,7,8-hexahydroquinazoline-4-thione (III), m. 199-201°. A mixture of 1 g. III and 10 cc. POCl3 was refluxed 1 hr., cooled and poured into ice, and extracted 3 times with CHCl3. The combined exts. were dried with anhydrous MgSO4 and evaporated to dryness in vacuo to yield 0.72 g. 4-chloro-2-phenyl-5,6,7,8-tetrahydroquinazoline (IV), m. 105-60° (EtOH). Similarly prepared were: 4-N[2-(4-morpholino)ethyl]amino-2-phenyl-5,6,7,8-tetrahydroquinazoline, 4-N-(2-N,N-dimethylaminoethyl)amino-5,6,7,8-tetrahydroquinazoline m.9 8-101°; 2-(4-chloro-phenyl)-4-N-(2-N,N-diethylaminoethyl)amino-5,6,7,8-tetra-hydroquinazoline; 2-(3-methylphenyl)-4-N-[2-(pyrrolidino)-ethyl]amino-5,6,7,8-tetrahydroquinazoline;2-(3,4-dimethoxy-phenyl)-4-N-[2-methyl-2-(1-piperazion))ethyl]amino-5,6,7,8-tetrahydroquinazoline; 2-(4-bromophenyl)-6-methyl-4-N-[3-(4-methyl-1 piperazino)propyl]amino-5,6,7,8-tetrahydroquinazoline; 4-N-[2-(N-ethyl-N-methylamino)ethyl]amino-2-(3-propyl)-5,6,7,8-tetrahydroquinazoline; 4-N-[2-(N-cyclopentyl-N-methylamino)ethyl]amino-2-(2-thienyl)-5,6,7,8-tetrahydroquinazo-line;2-benzyl-4-{2-[N-methyl-N-(2-phenylethyl)amino]ethyl}-5,6,7,8-tetrahydroquinazoline; 4-N-(2-N,N-dimethylaminoethyl)-2-phenyl-5,6-(1,3-propylene)pyrimidine; 4-N-(2-N,N-dimethylaminoethyl)-2-methyl-5,6,7,8-tetrahydroquinazoline; 2-isopropyl-4-N-[2-(4-morpholino)ethyl]-5,6,7,8-tetrahydroquinazoline and 4-(2-piperidinoethylamino)-5,6,7,8-tetrahydroquinazoline maleate, m.

L3 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

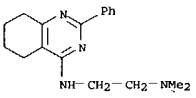
161-3°.

IT **17709-74-9P 17709-75-0P 17709-78-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 17709-74-9 CAPLUS
CN Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-5,6,7,8-tetrahydro-2-phenyl- (7CI, 8CI) (CA INDEX NAME)

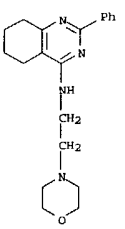


RN 17709-75-0 CAPLUS
CN Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-5,6,7,8-tetrahydro-2-phenyl-, dihydrochloride (8CI) (CA INDEX NAME)



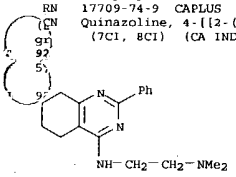
●2 HCl

RN 17709-78-3 CAPLUS
CN Quinazoline, 5,6,7,8-tetrahydro-4-[(2-morpholinoethyl)amino]-2-phenyl- (7CI, 8CI) (CA INDEX NAME)



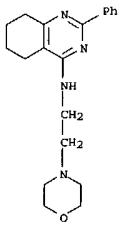
L3 ANSWER 43 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L3 ANSWER 44 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1964:476558 CAPLUS
DOCUMENT NUMBER: 61:76558
ORIGINAL REFERENCE NO.: 61:13308c-d
TITLE: Investigations in heterocycles. XVIII. The synthesis of 1,2-disubstituted 5,6,7,8-tetrahydro-4-quinazolinethiones
AUTHOR(S): Carney, Richard W. J.; Wojtkunski, Janice; DeStevens, George
CORPORATE SOURCE: Ciba Corp., Summit, NJ
SOURCE: Journal of Organic Chemistry (1964), 29(10), 2887-90
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:76558
GI For diagram(s), see printed CA Issue.
AB cf. CA 61, 9499g. Two methods for the synthesis of 1,2-disubstituted 5,6,7,8-tetrahydro-4-quinazolinethiones (I) are described: the reaction of 5,6,7,8-tetrahydro-2-phenyl-4-benzoxazinethione with various primary amines and the condensation of a N-monosubstituted enamine with an acyl isothiocyanate. Some chemical transformations of this heterocyclic system are discussed.
IT **17709-74-9**, Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-5,6,7,8-tetrahydro-2-phenyl- **17709-78-3**, Quinazoline, 5,6,7,8-tetrahydro-4-[(2-morpholinoethyl)amino]-2-phenyl- **92296-18-9**, Quinazoline, 4-hydrazino-5,6,7,8-tetrahydro-2-phenyl- **94113-12-9**, Ethanol, 2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]-
(preparation of)
RN 17709-74-9 CAPLUS
CN Quinazoline, 4-[[2-(dimethylamino)ethyl]amino]-5,6,7,8-tetrahydro-2-phenyl- (7CI, 8CI) (CA INDEX NAME)

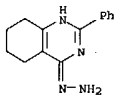


RN 17709-78-3 CAPLUS
CN Quinazoline, 5,6,7,8-tetrahydro-4-[(2-morpholinoethyl)amino]-2-phenyl- (7CI, 8CI) (CA INDEX NAME)

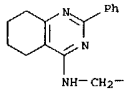
L3 ANSWER 44 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 92296-18-9 CAPLUS
CN Quinazoline, 4-hydrazino-5,6,7,8-tetrahydro-2-phenyl- (7CI) (CA INDEX NAME)



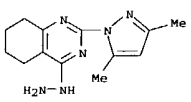
RN 94113-12-9 CAPLUS
CN Ethanol, 2-[(5,6,7,8-tetrahydro-2-phenyl-4-quinazolinyl)amino]- (7CI) (CA INDEX NAME)



L3 ANSWER 45 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1964:432502 CAPLUS
DOCUMENT NUMBER: 61:32502
ORIGINAL REFERENCE NO.: 61:5666h,5667a-b
TITLE: 2-(Pyrazol-1-yl)pyrimidine derivatives
INVENTOR(S): Shirakawa, Kenzo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 39004491		19640414	JP	19600308

GI For diagram(s), see printed CA Issue.
AB Manufacture of I, useful as antituberculous and antitumor drugs, was described. Thus, a mixture of 2 g. 3-(3,5-dimethylpyrazol-1-yl)-4-methyl-6-chloropyrimidine and 30% PhCH2NH2 solution (containing 2.9 g. PhCH2NH2) is boiled
1 hr., cooled, and extracted with Et2O to give 1.0 g. I (R1 = Me, R2 = H, R3 = benzylamino), m. 140-1° (dilute EtOH). Similarly prepared are the following I (R1, R2, R3, appearance, and m.p. given): Me, H, EtNH, powdery, 99-100° (ligroine); Me, H, NMe2, pale yellow needles, 87-8° (ligroine); Me, H, diethanolamino, needles, 75-7° (H2O); Me, H, piperidino, yellow oil, (b0.3 200-5°); Ph, H, hydrazino, needles, 206-7° (BuOH); (R1 R2 =) tetramethylene, hydrazino, needles, 182-3° (dilute EtOH); Me, H, hydrazino, needles, 183-4° (BuOH).
IT **92035-40-0**, Quinazoline, 2-(3,5-dimethylpyrazol-1-yl)-4-hydrazino-5,6,7,8-tetrahydro-
(preparation of)
RN 92035-40-0 CAPLUS
CN Quinazoline, 2-(3,5-di-methylpyrazol-1-yl)-4-hydrazino-5,6,7,8-tetrahydro- (7CI) (CA INDEX NAME)



L3 ANSWER 46 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1964:68217 CAPLUS
DOCUMENT NUMBER: 60:68217
ORIGINAL REFERENCE NO.: 60:12009h,12010a-h,12011a-c
TITLE: Pyrimidine derivatives. XII. 2-(1-Pyrazolyl)pyrimidines. 2
AUTHOR(S): Shirakawa, Kenzo; Tsujikawa, Teruaki
CORPORATE SOURCE: Takeda Res. Lab., Osaka, Japan
SOURCE: Takeda Kenkyusho Nenpo (1963), 22, 27-46
CODEN: TDKNAF; ISSN: 0371-5973
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Boiling of a mixture of 8 g. 2-(4-ethoxycarbonyl-5-methyl-1-pyrazolyl)-4-hydroxy-6-phenylpyrimidine, 70 cc. 4% NaOH, and 70 cc. EtOH for 30 min. gives 60.3% 2-(4-carboxy-5-methyl-1-pyrazolyl)-4-hydroxy-6-phenylpyrimidine, m. 320° (decomposition) (AcOH). Similarly prepared are 2-(4-carboxy-5-amino-1-pyrazolyl)-4-hydroxy-6-methylpyrimidine [m. 229° (decomposition) (dilute AcOH)], 2-(4-carboxy-5-amino-1-pyrazolyl)-4-hydroxy-5,6-tetramethylenepyrimidine [m. 250° (decomposition) (EtOCH2CH2OH)], and 2-(3,5-dimethyl-1-pyrazolyl)-4-hydroxy-5-carboxypyrimidine [m. 255° (decomposition) (MeOCH2CH2OH)] in 64%, 17%, and 34.4% yields, resp. They are dissolved in CHCl3 and treated with Cl or Br to give corresponding chlorinated or brominated products: (product, m.p., and % yield given): 2-(3,5-dimethyl-4-chloro-1-pyrazolyl)-4-hydroxy-5-chloro-6-methylpyrimidine, 248-51° (EtOH), 52.2; 2-(3,5-dimethyl-4-bromo-1-pyrazolyl)-4-hydroxy-5-bromo-6-methylpyrimidine, 246-8° (dilute AcOH), 83; 2-(3,5-dimethyl-4-bromo-1-pyrazolyl)-4-hydroxy-5-bromo-6-phenylpyrimidine, 150-1° (CHCl3), 83; 2-(3-methyl-4-bromo-5-phenyl-1-pyrazolyl)-4-hydroxy-5-bromo-6-phenylpyrimidine, 229-31° (PhMe), 67.3; 2-(4-ethoxycarbonyl-5-methyl-1-pyrazolyl)-4-hydroxy-5-bromo-6-phenylpyrimidine, 167-9° (dilute EtOH), 85.8%. 4-Hydroxy compds. are treated with POCl3 to give 4-Cl compds. Thus, the following I are prepared (R, R1, m.p., and % yield given): H, Me, 57° (dilute EtOH), 55; (RR1=) (CH2)3, 131-3° (C6H6-ligroine), 95.5; (RR1=) (CH2)4, 130-2° (ligroine), 58; H, Ph, 117-18° (dilute EtOH), 89. Reaction of I with NH2NH2.H2O gives II (R, R1, m.p., and % yield given): H, Me, 183-4° (BuOH), 72.5; (RR1=) (CH2)3, 1857° (dilute EtOH), 83.5; (RR1=) (CH2)4, 128-32° (dilute EtOH), 81.2; H, Ph, 206-7° (BuOH), 66. The synthesis of the following III is also reported (R, R1, R2, R3, R4, appearance, and m.p. given): Me, H, Me, NH2, Me, prisms, 114-16° (ligroine); Me, H, Me, NHPh, Me, plates, 112-13° (ligroine); Me, H, Me, NHCH2Ph, Me, needles, 142.5-3.5° (dilute EtOH); Me, H, Me, SMe, Me, needles, 103-4° (dilute dioxane); Me, H, Me, Me, NH2, needles, 120-3° (MeOCH2CH2OH); Me, H, Me, OH, Me, prisms, 288-9° (decomposition) (EtOH); H, CO2Et, Me, NH2, Me, plates, 153-5° (dilute EtOH); H, CO2Et, Me, NHPh, Me, prisms, 135-6.5° (80% EtOH); H, CO2Et, Me, NHCH2Ph, Me, plates, 143.5-5° (C6H6-ligroine); H, CO2Et, Ph, NH2, Me, prisms, 144-5° (dilute EtOH); H, CO2Et, NH2, NH2, Me, needles, 200-2° (70% EtOH); H, CO2Et, NH2, NHPh, Me, needles, 146-7° (dilute AcOH); H, CO2Et, NH2, NHCH2Ph, Me, leaflets, 148-50° (50% EtOH); H, CO2Et, NH2, OH, Me, needles, 298° (decomposition) (MeOCH2CH2OH); H, CN, NH2, NH2, Me, needles, 251-2° (80% EtOH); H, CN, NH2, NHPh, Me, needles, 2679° (EtOCH2CH2OH); H, CN, NH2, NHCH2Ph, Me, prisms, 203-5° (60% AcOH); H, CN, NH2, SMe, Me, needles, 239-40° (dilute dioxane); H, CN, NH2, OH, Me, needles, >300° (MeOCH2CH2OH). IV are also prepared (same data): Me, H, Me, H, Me, needles, 117-19° (80% EtOH); Me, H, Me, (R3R4=) (CH2)3, needles, 113-14° (ligroine); Me, H, Me, (R3R4=)(CH2)4, powder, 103° (dilute AcOH); Me, H, Me, H, Ph, needles, 153-4° (80%

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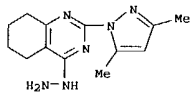
EtOH); H, CO2Et, Me, H, Me, prisms, 160-1° (dil. AcOH); H, CO2Et, Me, (R3R4=) (CH2)3, plates, 159.5-61° (C6H6); H, CO2Et, Me, (R3R4=) (CH2)4, needles, 130-3° (dil. AcOH); H, CO2Et, Me, H, Ph, needles, 165-6° (AcOH); H, CO2Et, NH2, H, Me, needles, 177-9° (AcOH); H, CO2Et, NH2, (R3R4=) (CH2)3, prisms, 182-3° (EtOCH2CH2OH); H, CO2Et, NH2, (R3R4=) (CH2)4, leaflets, 197-8° (BuOH); H, CO2Et, NH2, H, Ph, needles, 187-8° (AcOH); H, CN, NH2, H, Me, needles, 245-7° (AcOH); H, CN, NH2, (R3R4=) (CH2)3, powder, 249-50° (dil. AcOH); H, CN, NH2, (R3R4=) (CH2)4, needles, 225° (AcOH); H, CN, NH2, H, Ph, needles, 242-3° (AcOH). The following V are prepd. (R, R1, R2, R3, and m.p. given): 2-pyridyl, H, CO2Et, NH2, 93-5° (ligroine); 2-pyridyl, H, CN, NH2, 186-9° (EtCH2CH2OH); a, Me, H, Me, 165-7° (MeOCH2CH2OH); a, H, CO2Et, Me, 160-2° (MeOCH2CH2OH); a, H, CO2Et, NH2, >300° (MeOCH2CH2OH); a, H, CN, NH2, >300° (MeOCH2CH2OH); b, H, CO2Et, NH2, 216° (decompn.) (MeOCH2CH2OH); c, Me, H, Me, 104-5° (MeOCH2CH2OH); c, H, CO2Et, NH2, 132-5° (MeOCH2CH2OH); d, Me, H, Me, 106-9° (MeOCH2CH2OH); e, Me, H, Me, 123-4° (EtOH); f, Me, H, Me, 132-3° (EtOH); g, Me, H, Me, 143-5° (dil. EtOH); h, H, CO2Et, NH2, 130-1° (MeOH); i, H, CO2Et, NH2, 88° (EtOH); j, Me, H, Me, 237° (dil. EtOH); k, Me, H, Me, 68-70(EtOH); l, Me, H, Me, -(oil, b4 204°); m, H, CO2Et, NH2, 278° (decompn.) (MeOCH2CH2OH); o-MeOC6H4, Me, H, Me, -(oil. b14 161-4°); p-H2NO2SC6H4, Me, H, Me, 228-30° (MeOCH2CH2OH); m-HO3SC6H4, Me, H, Me, 313° (decompn.) (dil. EtOH); p-HO2CCH2C6H4, Me, H, Me, 151-2.5° (dil. EtOH); p-HO2CCH2C6H4, Me, H, Ph, 189-90° (dil. EtOH). The following VI are prepd. (R and m.p. given): n, 154-6° (EtOH); o, 95-7° (EtOH); p, 240° (decompn.) (MeSOMe); q, 244° (MeSOMe); a, 272° (MeSOMe); r, 220° (EtOH). 2-(1-Pyrazolyl)-4-hydroxypyrimidines were effective in inhibiting growth of Mycobacterium tuberculosis.

IT **92035-40-0**, Quinazoline, 2-(3,5-dimethylpyrazol-1-yl)-4-hydrazino-5,6,7,8-tetrahydro-
(preparation of)

RN 92035-40-0 CAPLUS

CN Quinazoline, 2-(3,5-di-methylpyrazol-1-yl)-4-hydrazino-5,6,7,8-tetrahydro-(7CI) (CA INDEX NAME)



L3 ANSWER 47 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:486834 CAPLUS
DOCUMENT NUMBER: 57:86834
ORIGINAL REFERENCE NO.: 57:4654h-i,4655a-f
TITLE: Syntheses with enamines. VIII. Heterocycles from enamine-isothiocyanate adducts
AUTHOR(S): Huenig, Siegfried; Huebner, Klaus
CORPORATE SOURCE: Univ. Marburg, Germany
SOURCE: Ber. (1962), 95, 937-43
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The adducts from enamines and isothiocyanates and their hydrolysis products, the β-carbonylthiocarboxamides, are excellent starting materials for the synthesis of heterocycles. Substituted amino groups can be introduced in this manner into difficultly accessible positions as demonstrated in the pyrazole and pyrimidine series. In 1 exceptional case a derivative of the previously unknown 3-azathio-4-pyrone was formed in place of the adduct. 1-Morpholino-1-cyclohexene (16.7 g.) in 15 cc. CHCl3 added dropwise with cooling and stirring during 45 min. to 32.6 g. BzNCS in 50 cc. CHCl3, cooled 1 h., stirred until no further temperature increase occurred, refluxed 0.5 h., and refrigerated overnight yielded 12.0-13.4 g. 2-phenyl5,6,7,8-tetrahydro-1,3-benzoxazine-4-thione (I), orange needles, m. 198-9° (HCONMe2) (all m.ps. are corrected); the tarry residue from the mother liquor gave some N-(morpholinothiocarbonyl)benzamide, m, 144-5°. I (2.43 g.) in 30 cc. refluxing Me2CO treated dropwise with 2.1 g. MeI in 5 cc. Me2CO, refluxed 0.5 h., cooled, and filtered gave 3.62 g. 4-methylthio-2-phenyl-5,6-tetramethylene-3-azapyrylium iodide (II), decomposed gradually above 150°; it evolved MeSH in moist air. II (2.3 g.) in 10 cc. refluxing EtOH treated dropwise during 5 min. with 10 cc. 2N HCl, refluxed 10 min., aerated, cooled, diluted with 20 cc. H2O, and filtered, and the residue repptd. from 15 cc. hot MeOH with 15 cc. H2O gave 1.12 g. N-benzoyl-2-cyclohexanonecarboxamide (III), m. 150-1.5°. III (1.021 g.), 5 cc. concentrated NH4OH, and 5 cc. EtOH refluxed 0.5 h. gave 552 mg. 4-hydroxy-2-phenyl5,6-tetramethylenepyrimidine (IV),. m. 238-9° (sealed capillary) (repptd. from HCONMe2 with H2O). II (5.0 g.) in 30 cc. refluxing MeOH treated dropwise during 5 min. with 10 cc. concentrated NH4OH, refluxed 0.5 h., cooled, diluted with H2O to incipient turbidity, and refrigerated overnight yielded 2.36 g. 4-MeS analog of IV, m. 118-19° (1:1 HCONMe2-H2O). 2-Ethyl-3-pyrrolidinoacrylic acid thioanilide (5.22 g.) and 1 cc. 90% N2H4.H2O heated in 25 cc. EtOH yielded 3.40 g. 3(5)-anilino-4-ethylpyrazole, rhombs, m. 113° (C6H6-ligroine). β-Morpholinothiocinnamic acid anilide (V) (3.24 g.), 15 cc. EtOH, and 1 cc. 90% N2H4.H2O refluxed 1.5 h., filtered, and diluted with a few cc.H2O gave 1.72 g. 3(5)anilino-5(3)-phenylpyrazole, plates, m. 152.5-3.5°; HCl salt, m. 167-8°. BzCH2CSNHPh (2.55 g.) in 15 cc. EtOH refluxed 1.5 h. with 1.62 g. PhNHNH2, diluted to turbidity with H2O, and filtered gave 2.4 g. 1,5-diphenyl-3-anilinopyrazole (VI), m. 154-5° (MeOH). V (3.24 g.) gave similarly 2.45 g. VI, m. 154.5-5.5°. 2-Morpholino-1cyclohexenethiocarboxanilide (VII) (6.0 g.), 35 cc. EtOH, and 1 cc. 90% N2H4.H2O refluxed 2 h., heated 15 min. with C, filtered, cooled, and diluted with 35 cc. H2O gave 2.95 g. 3-anilino-4,5-tetramethylenepyrazole (VIII), m. 169-70° (PhMe). 2-Cyclohexanonethiocarboxanilide (IX) (4.7 g.) gave similarly 2.76 g. VIII, m. 169-70°. 2-Morpholino-1cyclopentenethiocarboxanilide (5.75 g.), 30 cc. EtOH, and 1 cc. 90% N2H4.H2O refluxed 2 h., filtered, diluted with 2 vols. H2O, and refrigerated overnight yielded 2.75 g.

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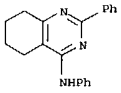
3-anilino4,5-trimethylenepyrazole (X), m. 163-4°. 2-Cyclopentanonethiocarboxanilide (4.38 g.) gave similarly 3.04 g. X. β-Morpholinothiocinnamic acid benzamide (3.52 g.) in 25 cc. EtOH refluxed 1 h. with 1 cc. 90% N2H4.H2O, filtered, treated with H2O to incipient turbidity, cooled, and filtered yielded 1.83 g. 3-benzamido-5-phenylpyrazole, m. 189-91° (MeOH). VII (3.02 g.) in 20 cc. EtOH refluxed 3 h. with 2.35 g. benzamidine-HCl, cooled, and filtered gave 1.47 g. 4-anilino-2-phenyl-5,6-tetramethylenepyrimidine (XI), m. 150-1° (ligroine). IX (2.33 g.) gave similarly in the presence of 0.015 mol NaOEt 1.35 g. XI, m. 150.5-1.5°.

IT **88828-40-4**, Quinazoline, 4-anilino-5,6,7,8-tetrahydro-2-phenyl-
(preparation of)

RN 88828-40-4 CAPLUS

CN Quinazoline, 4-anilino-5,6,7,8-tetrahydro-2-phenyl- (7CI) (CA INDEX NAME)



L3 ANSWER 48 OF 48 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:423207 CAPLUS
DOCUMENT NUMBER: 57:23207
ORIGINAL REFERENCE NO.: 57:4653e-i,4654a-h
TITLE: Syntheses with enamines. VII. Addition of isocyanates and isothiocyanates to enamines
AUTHOR(S): Huenig, Siegfried; Huebner, Klaus; Benzing, Erhard
CORPORATE SOURCE: Univ. Marburg, Germany
SOURCE: Ber. (1962), 95, 926-36
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:23207

AB cf. CA 55, 11398b. The addition of several enamines to various substituted isocyanates and iso- thiocyanates is described. The resulting adducts can be hydrolyzed smoothly to β-carbonyl(thio)carboxamides. Pyrrolidine (142 g.) and 50 g. powdered K2CO3 treated dropwise at -10° with 72 g. PrCHO, stirred 0.5 h. at room temperature, filtered, and distilled yielded 68 g.

1-pyrrolidino-1-butene (I), b12 57-9°. AcPh (120 g.) and 130 g. morpholine in 300 cc. PhMe refluxed 70 h. with 5 g. acidic montmorillonite catalyst K-10 with the azeotropic removal of H2O gave 101 g. 1-morpholino-1-phenylethylene (II), b0.1 86-9°. 1-Morpholino-1-cyclopentene (III) (15.3 g.), 25 cc. C6H6, and 9.9 g. BUNCO (IV) heated 2 h. under N at 60°, stirred 0.5 h. with 60 cc. 2.N HCl, the aqueous phase neutralized with solid No2CO3, saturated with NaCl, and extracted with C6H6, and the extract distilled yielded 10.3 g. 2-cyclopentanonecarboxylic acid butylamide, b0.05 103-5°; semicarbazone m. 206-9° (EtOH). 1-Morpholino-1-cyclohexene (V) (16.7 g.) and 9.9 g. IV heated 4 h. under N on the water bath, dissolved in 25 cc. CHCl3, and stirred with 55 cc. 2N HCl, and the aqueous phase worked up in the usual manner yielded 12.0-13.1 g. 2-cyclohexanonecarboxylic acid butylamide, b0.15 118-21°; semicarbazone m. 164-6°. III (30.6 g.) in 40 cc. Me2CO treated during 1 h. with stirring with 23.8 g. PhNCO and 10 cc. Me2CO, stirred, kept 1 h at room temperature, cooled 3 h. at 0°, and filtered gave 36.0-9.5 g. 2-morpholinocyclopentenecarboxanilide (VI), m. 122-7° (decomposition) (all m.ps. are corrected). VI (27.3 g.) in 125 cc. 2N HCl kept 2 h. and filtered gave 15.4 g. 2-oxocyclopentanecarboxanilide, leaflets, m. 90-2°, which heated 1 h. at 95°, change to prisms, m. 102-4°. V (16.7 g.) in 25 cc. Me2CO treated during 20 min. With 11.9 g. PhNCO, kept 1 h. at room temperature, 2.3-h. at 0°, and filtered gave 20.5-2.5 g. 2-morpholinocyclohexenecarboxamide (VII), m. 120-5°. VII (14.2 g.) in 60 cc. boiling MeOH treated dropwise with a few cc. 2N HCl, filtered, treated with HCl (total amount 30 cc.), cooled, and filtered gave 10.010.4 g. 2-oxocyclohexanecarboxanilide, m. 106-8° (3:1 cyclohexane-EtOAc). II (9.45 g.) in 30 cc. cyclohexane treated dropwise during 15 min. with 5.95 g. PhNCO in 5 cc. cyclohexane, heated 0.5 h. at 80°, cooled, and filtered, the residue (12.1 g.) boiled with 60 cc. MeOH, acidified dropwise with 2N HCl, filtered, and refrigerated overnight gave 8.45-8.90 g. BzCH2CONHPh, m. 105-7°. I (12.5 g.) in 20 cc. dry EtOAc treated dropwise with stirring during 45 min. with 11.9 g. PhNCO at about 30°, refrigerated over-night, and filtered yielded 14.5 g. 1-pyrrolidino-1-butenecar-boxanilide (VIII), prisms, m. 117-23° (decomposition) (repptd. from hot EtOAc with petr. ether). VIII (7.5 g.) dissolved with warming with 15 cc. EtOH and 15cc. 2N HCl and cooled yielded 3.0 g. EtCH(OCNHPh)CH(OH)OEt, needles, m. about 95-100° (EtOH-petr. ether). p-MeC6H4SO2NCO (19.7 g.) in 20 cc. CHCl3 added during 1 h. with stirring to 16.7 g. V and 25 cc. CHCl3 at 30-5°, stirred 0.5 h. at room temperature, treated dropwise with 50 cc. 2N HCl. and stirred 0.5.h., the CHCl3 layer evaporated, and the oily residue refluxed 0.5 h. with C in 45 cc. C6H6, filtered, and refrigerated over-night yielded 18 g.

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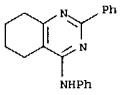
N-(p-MeC6H4SO2) deriv. of VII, m. 125-7° (C6H6). III (30.6 g.) in 75 cc. MeOH treated dropwise with stirring during 0.5 h. with 27 g. PhNCS in 20 cc. MeOH, refluxed 1 h., and refrigerated overnight gave 47.5-9.5 g. 3-morpholino-1-cyclopentenethiocarboxanilide (IX), m. 115-19° (decompn.) (MeOH). IX (5.0 g.) in 20 cc. refluxing EtOH neutralized dropwise with 2N HCl and cooled gave 3.2 g. 2-cyclopentanonethiocarboxanilide, m. 96-7° (cyclohexane-EtOH). V (33.5 g.) (33.5 g.) in 75 cc. MeOH and 27 g. PhNCS refluxed 1.5 h. and refrigerated overnight yielded 45.8-50.2 g. 2-morpholino-1-cyclohexene-thiocarboxanilide (X), m. 125-9° (decompn.) (MeOH). X (4.8 g.) in 30 cc. refluxing EtOH neutralized slowly with about 10 cc. 2N HCl, dild. with 3-4 cc. H2O, and refrigerated overnight gave 2.3 g. 2-cyclohexanonethiocarboxanilide, m. 84-9° (decompn.) (cyclohexane-EtOAc). II (9.5 g.), 30 cc. EtOAc, and 6.75 g. PhNCS refluxed 1 h. and cooled yielded 12.5 g. β-morpholinothiocinnamic acid anilide (XI), m. 157-8° (EtOAc). XI (3.24 g.) in 20 cc. EtOH acidified dropwise with 2N HCl, treated with a few drops H2O, and refrigerated overnight gave 2.4 g. BzCH2CSNHPh, m. 80-3° (1:1 EtOH-H2O). I (12.5 g.) and 25 cc. EtOAc treated with stirring during 20 min. dropwise with 13.5 g. PhNCS, refluxed 0.5 h., and refrigerated overnight gave 17.5 g. 1-pyrrolidino-1-butene-2-thiocarboxanilide, yellow plates, m. 106-9° (decompn.) (EtOH). II (18.9 g.) in 50 cc. cyclohexane treated dropwise during 45 min. with stirring with 16.3 g. BzNCS in 25 cc. cyclohexane and filtered after 1 h. gave 26.4 g. N-benzoyl-β-morpholinothiocinnamamide (XII), m. 161-4°. XII (17.6 g.) in 200 cc. EtOH treated slowly dropwise with 5.5 cc. concd. HCl, refluxed 0.5 h., cooled, and filtered yielded 12.3 g. BzCH2CSNHBz (XIII), m. 140-2° (1:1 EtOH-H2O). XIII (5.0 g.), 25 cc. EtOH, and 10 cc. concd. NH4OH refluxed, treated with a small amt. C, refluxed 1 h., filtered, ditd. to incipient turbidity with H2O, cooled, and filtered, and the residue boiled briefly with 35 cc. 2N HCl, cooled, and filtered gave 3.1 g. BzCH2-CONHBz, m. 168-9° (in sealed capillary) (repptd. from HCONMe2 with H2O). III (7.7 g.) in 50 cc. ligroine treated dropwise with stirring during 45 min. with 8.15 g. BzNCS in 10 cc. ligroine at 35-40°, stirred 0.5 h. at room temp., and filtered gave 13.2 g. N-benzoyl-2-morpholinothiocar-boxamide (XIV). XIV (3.16 g.) in 25 cc. hot 1:1 EtOH-H2O treated dropwise slowly with concd. HCl to acidity, heated to boiling, and refrigerated overnight yielded 1.63 g. N-benzoyl-2-cyclopentanonethiocarboxamide, yellow needles, m. 91.5-2.5° (MeOH).

IT **88828-40-4**, Quinazoline, 4-anilino-5,6,7,8-tetrahydro-2-phenyl-
(preparation of)

RN 88828-40-4 CAPLUS

CN Quinazoline, 4-anilino-5,6,7,8-tetrahydro-2-phenyl- (7CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	230.24	385.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-33.60	-33.60

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